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Argonne National Laboratory

APPLIED MATHEMATICS DIVISION SUMMARY REPORT

July 1, 1966 through June 30, 1967

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ANL-7418
Mathematics and Computers
(TID-4500)
AEC Research and
Development Report

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

APPLIED MATHEMATICS DIVISION
SUMMARY REPORT

July 1, 1966 through June 30, 1967

Wallace Givens, Division Director

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PREFACE

The Applied Mathematics Division has a twofold objective:

1) to conduct research in applied mathematics, numerical analysis, theory and practice of computation, and design of computer and information processing equipment;

2) to provide mathematical, computer programming, and computational support for the research and development programs of the Laboratory.

Members of the Consultation and Research Section carry out their own independent research in various aspects of mathematics and programming. They are also available to assist laboratory personnel by mathematical consultation, in problem formulation, and in selection of appropriate mathematical and numerical techniques, and to carry out analysis of problems. The functions of the Computer Engineering Section are (applied) computer engineering research, and the development and design of computers and information-processing systems having special application to the nuclear sciences.

The Analog group is prepared to assist in the formulation, programming, and running of problems for the Analog computer or to accept the problem and carry out these services entirely within the group.

The Digital Computing Center operates the central computing facility and provides systems programming support for it. Through its Systems Programming Section, the Center engages in advanced systems development aimed at the enhancement of the services of the computing facility and at advancement of computer systems technology. Members of the Computing Center's Applied Programming Section work with scientists from other divisions in formulating and defining problems for solution on digital computers. Applied programmers then carry out the necessary programming and documentation to achieve the ends specified in the program design.

APPLIED MATHEMATICS DIVISION

Organization Chart

July 1, 1966 through June 30, 1967

Director: W. Givens

Executive Assistant: D. A. Davis
Staff Assistant: R. E. King

Secretaries: M. Johnson, E. Dreifuerst(T), E. Fletcher(E), D. Haight, S. Mueller, G. Ramsey(E)
Receptionist: L. Zimmerman

Publications and Reports

Assistant Director: R. F. King
General Codes Distrib.: *W. J. Cody

Secretaries: M. Jedlicka, G. Krause

Argonne (Reactor) Code Center

Head: *M. Butler
Secretary: N. Kazich
L. Ranzini(E)
M. Legan

DIGITAL COMPUTING CENTER

Head: W. Cowell
Assistant Heads: J. Gabriel, B. Garbow, M. Storm
Secretary: K. Hostert

DIGITAL OPERATIONS

Operations Manager: C. LeVee
Asst. Oper. Manager: W. Greenhow
Asst. Oper. Manager: R. VanBuskirk

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A. Johnson(E)
N. Koca(E)
D. Koenig
S. Morris(E)
R. Sweeney(E & T)

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E. Overall(E)
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Central Machine Operations

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D. Greenwood(T) *Shift Leaders*
T. Unger

J. Barton
R. Bilshausen
A. Burger(E)
C. Caruthers(E)
J. Clapp
R. Clinkert(E)
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B. Dudek(T)
M. Gordon(T)
J. Guderian(T)
S. Halcarz(E & T)
R. Jarka

W. Jones(E)
C. Kilty
M. Lawler(E)
R.
M.
J.
R.
J.
B.
J.
R.
K.
E.
R.
A.

Remote Station Operation

J. Beck
++L. Douglas
H. Krejci
L. Michel(T)
J. Nelson
L. Nelson

SYSTEMS PROGRAMMING

Clerical: J. Beumer

Standard System Maintenance

J. Ohde, *Leader*
D. Brooks, *User Consultant*
H. Carlson
*W. Greenhow
A. Sandrin
++D. Snider(E & T)
J. Wenger

System 360 Development

R. Logan(E), *Leader*
D. Carson(E)
K. Dritz(E)
M. Fisherkeller(T)
A. Hirsch(E)
A. Joseph
R. Julke
R. Krupp
C. Smith(E)

APPLIED PROGRAMMING

Exec. Secretary - Assignment & Review Board: M. Prastein(E)
Secretarial: *K. Hostert
Production Services: S. Katilavas

Experimental Science

D. Woodward, *Leader*
J. Anderson
J. Gregory
J. Gvildys
J. Herman
A. Strecok

Engineering & Applied Systems

*B. Garbow, *Acting Leader*
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R. Clark
C. Harrison
N. Jesse
R. Mueller
P. Pennock
J. Scherer
W. Snow

Theoretical Physics & Chemistry

*D. Phillips, *Scientific Leader*
C. Chamot, *Group Manager*
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W. Hafner(T)
M. Howe
M. Kraimer(T)
A. Lent(T)
M. Matthies
K. Paciorek(E)
F. Taraba
S. Zawadzki

Reactor Theory & Development

*G. Leaf, *Scientific Leader*
S. Sparck, *Group Manager*
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B. Chandler
G. Duffy
H. Greenspan
D. Homewood(E)
G. Jensen
L. Just
J. Kaganove
A. Kennedy
L. Meyer
A. Rago
P. Walker
S. Welbourn(E)
J. Zapatka(E)
J. Zeman(T)

CONSULTATION AND RESEARCH

MATHEMATICAL ALGORITHMS

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M. Butler
W. Cody
*W. Cowell
*W. Givens
*R. F. King
G. Leaf
J. Lyness(E)
D. MacLaren
J. Reynolds
G. Robinson(T)
F. Stetter(E)
D. Taylor
++R. Thomas
L. Wos

MATHEMATICAL ANALYSIS

I. Abu-Shumays
E. Bareiss
P. Brockwell
R. Buchal
J. Cook
T. Hughes
J. Moyal
D. Phillips
V. Pless(E)
++J. Pool
W. Smith(E)
++J. VanRyzin
*D. Woodward

COMPUTER ENGINEERING

D. Jacobsohn, *Head*
L. Amiot
R. Aschenbrenner
D. Hodges
F. Salter
C. Shelman
R. Vonderohe

Technical Support:

W. Ball(E)
R. Barr
J. Becker
R. Foster
H. George
J. Haasl
B. Kroupa
F. Sato
R. Schwanke
N. Sobol
V. Tantillo
R. Wehman
G. Wittmus

Drafting:

V. Grynczyk

PROGRAMMING DEVELOPMENT

Logical Methods

*L. Wos
L. Shalla

Numerical Methods

*W. Cody, *Leader*
N. W. Clark
K. Hillstrom
D. Jordan
++V. Klema(E)
*J. Lyness
E. Thieleker

Partial Differential Equations

*D. Taylor
W. R. Wessel(E)

ANALOG COMPUTING CENTER

F. Morehouse, *Leader*
++H. Crosby
A. Winiecki

Technical Support

F. Maletich
W. Scott(T)

(E) Entered during
(T) Terminated dur iod.
* Supplementary .

++ Special Arrang

H. A. Crosby:	Visiting from Southern Illinois University.
L. Douglas:	Educational leave.
V. Klema:	Part-time.
J. Pool:	On leave in Europe to 9/1/67.
D. Snider(T):	Temporary joint appointment with Western Michigan University.
R. J. Thomas:	Visiting from DePauw University.
J. VanRyzin:	On leave at Stanford University to 9/1/67.

ORGANIZATION CHART (Cont'd.)

TEMPORARY PROGRAM

SUMMER 1966

Resident Research Assoc.

W. Gautschi
C. W. Gear
A. Ramsay
P. Slepian
C. H. Wilcox
C. R. Williams

Resident Student Assoc.

J. B. Cohen
R. D. Nussbaum
D. D. Porter
J. B. Rizza
L. Sanathanan

Student Aides

J. M. Carter
D. A. Hanson
J. A. Marentic
M. Megson
D. M. Rocke
R. Toussaint
E. R. Williams
J. G. Williams

LONGER TERM

Staff

I. Abu-Shumays
J. Boyle
W. Smith
F. Stetter

SUMMER 1967 (To June 30)

Resident Research Assoc.

R. Blum
W. Gautschi
B. Levinger

Resident Student Assoc.

D. Johnson
D. M. Rocke

Student Aides

A. Bradley
R. Dreyer
J. Glover
L. Leibovich
J. Marentic
J. Rozema

CONSULTANTS

G. Birkhoff, Harvard University
W. W. Boone, University of Illinois
J. M. Boyle, Northwestern University
H. Cohn, University of Arizona
R. Courant, New York University
M. J. Flynn, Northwestern University
L. D. Fosdick, University of Illinois
C. W. Gear, University of Illinois
M. Golomb, Purdue University
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H. C. Thacher, University of Notre Dame
R. S. Varga, Case Western Reserve University
C. H. Wilcox, University of Arizona
A. Wouk, Northwestern University

COMPUTER SYSTEMS AND LANGUAGES

Installation of IBM System 360 Computer Complex

The Applied Mathematics Division's large, new digital computer, an IBM System/360 with Model 75 and Model 50 processors, was installed on the scheduled date of June 30, 1967. The two processors of the 360 complement each other for maximum efficiency. While the very fast Model 75 concentrates on actual computation, the Model 50 handles peripheral activities such as input/output, accounting, and control of the over-all operation. In addition to its high speed, the new system has a much larger memory than any of its Argonne predecessors. The memory hierarchy includes two levels of magnetic cores, a magnetic drum, sixteen magnetic disks, two data cells (each consisting of many short strips of magnetic tape), and six magnetic tape units.

Besides conventional printers, card readers, and card punches, there are eight character-display units and will be an interactive graphic display unit and a graphic film recorder. A variety of software programs that enable users to communicate more easily with the machines were delivered as part of the entire system.

The testing program for the system is to consist of both specific hardware tests and total system operations tests. Mainframe tests are to be conducted to verify such items as the instruction repertoire, memory protection features, operation interrupts, and arithmetic timing. Tests have been designed to check exhaustively the operating characteristics of all peripheral devices; this includes the unit record devices, the 2314 disks, the 2301 drum, and the 2321 data cells. In addition, there will be a controlled reliability test on the 2321 data cells.

System operations testing is to consist of running in a production environment a library of 71 known programs and the regular production job stream. The library contains three types of programs: programs which exercise the compilers of the system, computational programs with known input and output, and a set of programs which had revealed faults in previous releases of the operating system.

ARGONNE NATIONAL LABORATORY
APPLIED MATHEMATICS DIVISION
S/360 DEVELOPMENT CONFIGURATION

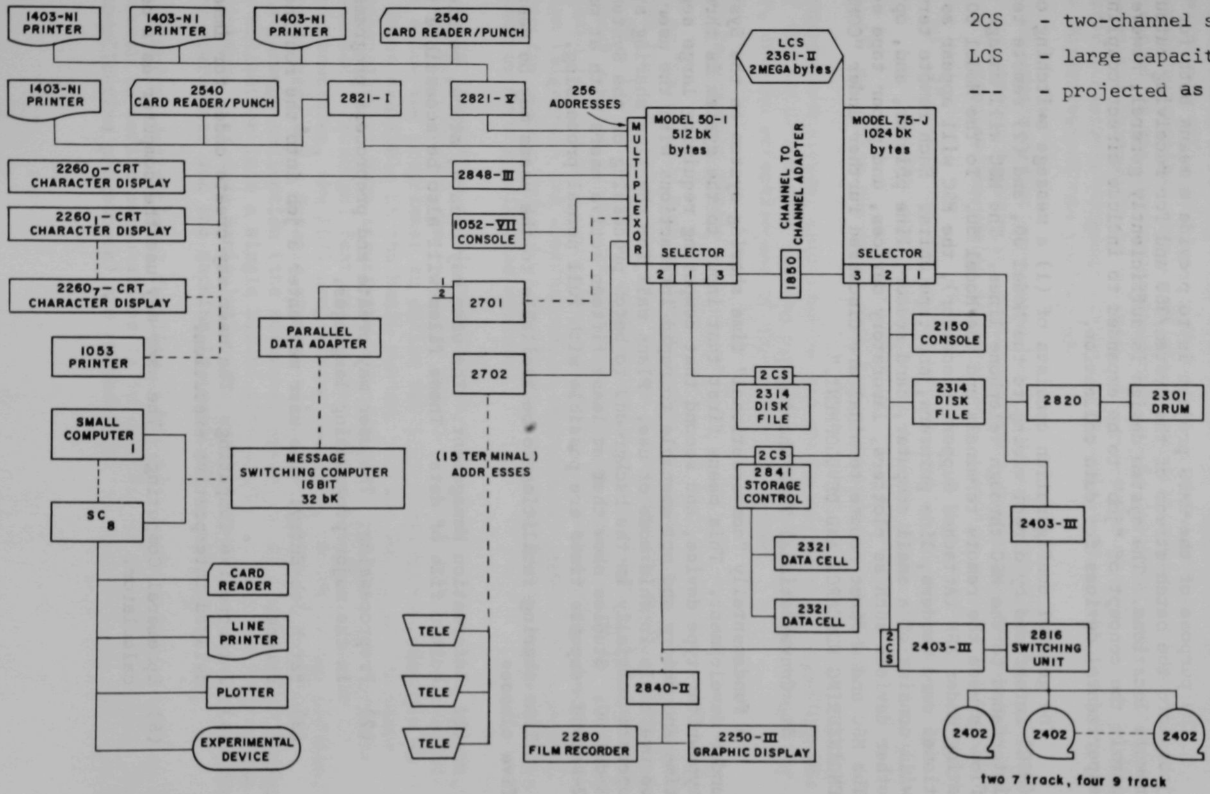
Legend

512bK = 512 times 1024 bytes

2CS - two-channel switch

LCS - large capacity storage

--- - projected as of 6/30/67



Development Projects for the IBM System/360

A. Remote Access Data System (RADS)

The purpose of the RADS project is to provide a means both for entering jobs into the batch stream of the System/360 and for receiving output at remote locations. The system design is sufficiently general, however, to permit the concept of "job" to be expanded to include direct coupling to experimental devices for data collection.

The general configuration consists of (1) a message switching computer (MSC) interfaced by direct wiring to the Model 50, and (2) remote terminals interfaced to the MSC through telephone lines. The MSC will manage the data flow between the remote terminals and the Model 50. To the Model 50, operating under ASP (Attached Support Processor), the MSC will appear as additional card readers, line printers, and tape units. Each remote terminal will consist of a small computer, card reader, line printer, and, optionally, other devices such as plotters, laboratory devices, and paper tape equipment. The MSC and a first remote terminal are discussed further under "COMPUTER ENGINEERING RESEARCH AND DEVELOPMENT."

B. Conversational Time Sharing

A fundamentally "conversational" time sharing system on the System 360 is under development. This means first that input to the system is through a typewriter-type device, and second that computing requiring large segments of time and memory and not amenable to rapid interactions with the user will not be available in this mode of use. Plans call for the time sharing system to operate initially in the background to batch processing on the System 360 Model 50. Studies show that at least fifteen active users with at most 2-second response times are possible with full normal processing.

Time sharing facilities to be available to the users may be described in five classes.

(1) Information Management: The user may create, store, retrieve, or edit a file of data. These files will also be accessible to batch jobs.

(2) Preprocessing: The user may create and preprocess programs written in the major programming languages.

(3) Batch Job Entry: The user may enter a job into the routine job stream.

(4) Interpretive Computing: The user may create codes for immediate or delayed interpretive execution.

(5) Ephemeral Computing: The user may use the computer as a desk calculator.

C. Computer Utilization and Systems Design

One of the principal unsolved problems in computer management, especially at scientific computing centers, is the measurement in quantitative terms of the efficiency of the computing process and the effectiveness of the computing complex relative to the needs of the users. A system now being developed in the Applied Mathematics Division will include 1) a statistical monitoring program to be an integral part of the system, and 2) a set of statistical analysis programs for analyzing the collected data. The immediate objectives of the project are to

a) evaluate the performance of the internal logic of the software system in allocating the resources of the computer to the required computing task;

b) determine how the system is affected by the Argonne job mix and to describe parametrically the job stream of Argonne; and

c) determine the spare capacity of the computing system.

With appropriate analyses, quantitative judgements may be made regarding the design of the batch and time sharing systems, potential needs for computing equipment, and the effectiveness of the computing center.

Extendible Programming System

EPS, or "Extendible Programming System," is a general purpose programming system for the larger computers in the IBM System 360 series, excluding the Model 67. EPS is being developed as a research project to test out various ideas related to the design of programming systems. It is, however, also intended for use as a production system in the area of non-numerical computation (algebraic and combinatorial computations, symbol manipulation, etc.), both for coding individual application programs and as a base for the construction of more specialized systems.

EPS is an integrated combination of two subsystems: 1) a basic system, in which all EPS programs can be coded, and 2) a set of definitional facilities that allow the programmer to define new high-level system elements in terms of those available in the basic system. In the design of the basic system, generality of data structures and of dynamic program structure has been emphasized. Principal features in this regard are the inclusion of arrays and structures, the PL/I programming language, recursive and parallel use of procedures, and a dynamic storage allocation system that includes relocating garbage collection (the automatic detection of free storage blocks and their collection into a single block) with almost no restrictions on the use of pointers. For data manipulation the basic system provides the standard elementary operations and the machine instructions of the System 360.

The principal definitional facility in EPS is a macro language that enables the programmer to define computations to be carried out at compile time. EPS macros (compile-time procedures) are conventional in that they are executed by translating a sequence of parametric statements, the parameters (which are macro variables) being interpreted according to their current values. However, the EPS macro facility goes beyond that in other systems in the degree to which macro processing is integrated with the compilation process, and the generality of the macro language. In particular, macros may interrogate the attributes of variables, declare variables and directly bind them to macro variables without having to generate intermediate identifiers, perform all types of arithmetic and logical operations, use arrays, call each other recursively, and do list processing with the system handling garbage collection.

The definitional facilities in EPS also include a method for defining new pseudo data types which are represented by real data types (i.e., data types in the basic system). Existing operators may be extended to act on the new data types and new operators may be defined. EPS also includes features to facilitate production and extension of the basic system.

At the present time the precise specification of EPS is just being completed, and the implementation is just beginning. A preliminary compiler will be coded in PL/I and this will be used to compile the system run-time routines and the regular compiler, all of which are written in the EPS language.

Numerical Methods

The FORTRAN IV library of functions supplied to Argonne by the International Business Machines Corp. on delivery of its System/360 Model 50 has been examined in detail for accuracy and speed. Tests included comparison against computations in a higher precision using large samples of random numbers. In the case of double-precision routines this involved communication with the CONTROL DATA 3600 via magnetic tape. Based largely on the results of this certification effort, the FORTRAN IV library is being extensively modified by scientists at Argonne, at NASA Lewis Research Center, and at The University of Chicago.

Much of the subroutine library for the CONTROL DATA 3600 has been converted for the new machine. New routines are constantly being developed for both machines, especially in the areas of matrices, quadrature, and special functions.

ERROR COMPARISONS FOR FORTRAN IV LIBRARY SUBROUTINES TO COMPUTE x**y, i.e., $x^y = \exp(y\ \ell n(x))$, SHOWING IMPROVED ACCURACY OF THE ARGONNE SUBROUTINE

Argument range for random arguments	Frequency of difference $\lvert x^y \text{ (computed)} - x^y \text{ (true)}\rvert$ in units of least significant bit of result									
	0	1	2 bits	3 bits	4 bits	5 bits	6 bits	7 bits	8 bits	other
Original IBM Subroutine										
$2^{-4} \le x \le 2^4, \lvert y\rvert \le 4$	501	443	432	297	202	107	18	0	0	0
$2^{-16} \le x \le 2^{16}, \lvert y\rvert \le 16$	129	171	189	238	312	371	294	219	75	2
$2^{-32} \le x \le 2^{32}, \lvert y\rvert \le 8$	145	184	190	218	247	295	254	204	125	138
$2^{-64} \le x \le 2^{64}, \lvert y\rvert \le 4$	111	165	181	166	197	258	285	298	210	129
$2^{-8} \le x \le 2^8, \lvert y\rvert \le 32$	100	123	197	210	255	364	282	277	156	36
$2^{-4} \le x \le 2^4, \lvert y\rvert \le 64$	109	136	184	204	200	303	328	230	184	122
Corresponding Argonne Subroutine										
$2^{-4} \le x \le 2^4, \lvert y\rvert \le 4$	1933	67	0	0	0	0	0	0	0	0
$2^{-16} \le x \le 2^{16}, \lvert y\rvert \le 16$	1771	226	3	0	0	0	0	0	0	0
$2^{-32} \le x \le 2^{32}, \lvert y\rvert \le 8$	1906	94	0	0	0	0	0	0	0	0
$2^{-64} \le x \le 2^{64}, \lvert y\rvert \le 4$	1938	62	0	0	0	0	0	0	0	0
$2^{-8} \le x \le 2^8, \lvert y\rvert \le 32$	1609	357	44	0	0	0	0	0	0	0
$2^{-4} \le x \le 2^4, \lvert y\rvert \le 64$	1392	440	140	28	0	0	0	0	0	0

Automatic Computation of Data Descriptions

In most machine-independent computer programming languages, a program is specified by giving two kinds of information: procedures for processing data, and descriptions of the type of data to be processed. In several recent languages (for example, PL/I and various proposals for ALGOL X) which provide for an elaborate variety of data types, the data-descriptive information may form a substantial portion of a typical program. However, it is intuitively evident that much of this information is redundant, i.e., that the nature of the data being processed is implicit in the procedures for processing it.

This had led to an attempt to devise algorithms for automatically computing data descriptions for procedures. A recently developed algorithm accepts a procedure in the well-known list processing language LISP and a description of its input data, and produces a description of the output data, as well as any intermediate data within the procedure. Thus, for example, the algorithm can be given a LISP procedure which converts a finite set (list) of symbols into the set of all subsets of the original set, and it will produce a data description showing that the output of the procedure must be a set of sets of symbols. Although the algorithm is capable of handling non-trivial procedures, it must be emphasized that major extensions will be necessary before it can be applied to a realistically complex programming language.

Throughout this development, data descriptions have been treated as a special case of recursive set definitions, in which the set being defined is a set of data. In general, such a definition defines a set (or a finite sequence of sets) as the limit of the sets formed by repeated application of some function to the empty set. Several new theorems show various ways these definitions can be transformed without changing the set being defined. These theorems may also be applicable to other set-definition methods that are used in non-numerical computing and that can be viewed as recursive set definitions; for example, the definition of a set of well-formed strings by a context-free grammar, or the definition of a set of logically valid statements by a set of axioms and inference rules.

SATCOPS System

SATCOPS is a support system residing in a CONTROL DATA 160-A computer directly coupled to a CONTROL DATA 3600 computer used as the main processor.

Using a large shared disk file as the intermediate input/output storage device, its major function is to reduce turnaround time while increasing throughput. This is achieved by eliminating from the main processor most support functions, such as job scheduling, input/output device allocation, card reading, printing, and card punching, and performing these tasks in the smaller (160-A) computer.

In a limited sense SATCOPS can be considered a time sharing system. Simultaneously with communicating to the SCOPE monitor program on the 3600, SATCOPS may be printing output from up to three different jobs and entering a fourth job into the system via a card reader. Associated operator messages are routed to a console typewriter attached to the 160-A computer, thereby reducing the amount of message reporting required on the main processor console typewriter. Logging of the input jobs, job scheduling messages, and tape mounting messages on the typewriter provide the operator a convenient running status report.

Servicing the interface between the two computers receives highest priority, while driving of the input/output devices is handled in a sequential manner. Jobs are scheduled for the 3600 from three input queues in a simple priority sequence. Two queues are on the disk file, while a third resides on magnetic tape (standard input device). Setup jobs (requiring mounting of programmer tapes) when ready are run first; otherwise, non-setup jobs fill in. If either of these two queues is temporarily empty or not ready, then the system automatically resorts to magnetic tape for backup input. In this manner improved throughput is realized by minimizing operator intervention and by reducing operator delays (a setup job is scheduled only when all tapes for it have been pre-mounted).

The built-in priority scheduling can be altered slightly through manual operator techniques. Non-setup jobs are forced to fill in if an operator chooses not to respond to tape mounting requests. Also, under operator control, the option of selecting input jobs from magnetic tape only is provided, with the possibility of returning to the normal mode at any time.

Macro-Programming

A language and CONTROL DATA 3600 computer program called MACRO-FORTRAN has recently been developed. It enables a programmer to write specifications for generating sequences of FORTRAN-language statements and to incorporate these sequences into his FORTRAN program in a natural fashion. (A macro-instruction is essentially a procedure for generating a sequence of statements in some algorithmic language, and can be thought of, for example, as a shorthand way of writing complicated FORTRAN statements.) Although in principle such a program, or translator, could be incorporated directly into FORTRAN itself, the present implementation has been made in the form of a preprocessor that generates input for the FORTRAN compiler. The MACRO-FORTRAN translator is itself written entirely in the 3600 FORTRAN language. The FORTRAN language generated by MACRO-FORTRAN can be for the 3600 or for other machines.

Digital computer programs are usually written as statements in an algorithmic language such as FORTRAN and then translated by means of another program called a "compiler" into a sequence of instructions in the language of the computing machine itself. Such instructions may then or later be executed to produce meaningful results from given sets of data, although the exact sequence of computations executed may vary with the specified input parameters.

One common device used in the efficient writing of programs is the closed subroutine, normally an algorithm for carrying out a task required more than one place in a program. The program for a closed subroutine is split off as an independent entity from the main program, rather than being incorporating each place it is used, to save machine memory space (since only one copy need be stored), and to reduce tedious clerical work by the programmer. When the sequence of computations to be performed depends only on the value of a small number of arguments that all vary dynamically at execution time, use of the closed subroutine is usually a very efficient technique. However, when some of the parameters depend only on the point in the main program at which the task must be performed (and therefore remain constant during execution time), or several parameters with no simple interrelations must be communicated to the subroutine, then the use of the macro-instruction may substantially enhance efficiency.

Peripheral Support and Microwave Service

A complete revision of the CONTROL DATA 160-A Standard Peripheral Processor (SPP), a comprehensive input/output package, has been completed and placed into operation. The principal tasks supported by the program include preparation of SCOPE (the standard CONTROL DATA 3600 operating system) input tapes for the CONTROL DATA 3600, printing of SCOPE output tapes, and punching of SCOPE standard punch tapes. Additional facilities permit other utility tasks, such as card-to-printer, card-to-punch, card-to-tape, tape-to-tape, tape-to-printer, and tape-to-punch. A restricted form of tape testing can be accomplished, although this is practical only when the number of tasks is light. Up to four tasks may be operating concurrently. In conjunction with input/output processing, the SPP program has facilities for microwave communications between stations located in the High Energy Physics (HEP) and Applied Mathematics (AMD) Buildings.

Since the microwave link is technically used as a vehicle for tape-to tape copying between the two sites, the tape-to-tape processor in SPP is used for processing the data transmitted.

Input jobs to be run on the 3600 are submitted by HEP users to the 160-A operator in the HEP Building, who will prepare an input tape via the card-to-tape operation. A microwave telephone hookup is used to establish feasibility of transmission, and the operation is initiated when both stations are mutually ready. Each station is capable either of receiving or of transmitting. Normal practice is to transmit input tapes from the HEP Building to the AMD Building and to send output tapes from the 3600 in AMD to HEP.

The transmission schedule currently is on an informal basis. At the discretion of the operator in the HEP Building, input tapes are sent whenever a sufficient number of jobs have been collected or if the elapsed time is 2 to 3 hours. This has insured the HEP users between 2 and 3 turnarounds per day. Transmission reliability has been high and the length of transmitting is relatively short, so that a re-transmission is very practical in the event of error.

New Library Routines

ANL B156S ARSIN	W. J. Cody	360 routine to evaluate the arcsine or arccosine of a single precision floating-point variable
ANL B157S SIN/CØS	K. Hillstrom	360 FORTRAN routine for the sine and cosine
ANL B251 SINH	K. Hillstrom	3600 routine to evaluate the hyperbolic sine SINH(X) or cosine COSH(X) of a real floating-point argument X
ANL B353S ALØG	N. W. Clark	360 routine to compute the natural (or base 10) logarithm of a single precision floating-point number
ANL B355S DLØG	N. W. Clark	360 routine to compute the natural (or base 10) double precision logarithm of a double precision floating-point argument

ANL C363	FRNLCX	K. Hillstrom	3600 routine to evaluate the Fresnel integrals $$C(X) = \int_0^X \cos(\pi/2\ t^2)\ dt$$ or $$S(X) = \int_0^X \sin(\pi/2\ t^2)\ dt$$ for a real floating-point argument X
ANL C364	CGAMMA	K. Hillstrom	3600 routine to evaluate the gamma function $\Gamma(z)$ of a complex floating-point argument z
ANL C365S	ALGAMA	K. Hillstrom	360 routine to evaluate the natural log of the gamma function of a real, single precision, floating-point argument x
ANL D150S	HAVIE	K. Hillstrom	360 FORTRAN routine to evaluate the definite integral of a function (integrand) of a real single or double precision floating-point argument x over an interval [a,b]
ANL D151S	ROMBRG	K. Hillstrom	360 FORTRAN routine to evaluate the definite integral of a function (integrand) of a real single or double precision floating-point argument x over an interval [a,b]
ANL D152	CHEBINT	K. Hillstrom	360 routine to evaluate the definite integral of a function (integrand) of a floating-point argument X over an interval [a,b]
ANL D153	DRØMB	K. Hillstrom	3600 FORTRAN routine to evaluate the definite double integral $\int_{a_1}^{b_1} \int_{a_2}^{b_2} f(x,y)dxdy$ of a function (integrand) of real single precision floating-point arguments x and y over the rectangle $a_1 \leq x \leq b_1$, $a_2 \leq x \leq b_2$
ANL D153S	DRØMB	K. Hillstrom	360 FORTRAN routine to evaluate the definite integral $\int_{a_1}^{b_1} \int_{a_2}^{b_2} f(x,y)dxdy$ of a function (integrand) of real double precision or single precision floating-point arguments x and y over the rectangle $a_1 \leq x \leq b_1$, $a_2 \leq y \leq b_2$

ANL D154	CMQUAD	K. Hillstrom	3600 FORTRAN routine to evaluate the definite integral $\int_a^b f(x)dx$ of a function (integrand) of a real single precision floating-point argument x over the interval $a \leq x \leq b$
ANL D155	SIMP	K. Hillstrom	3600 FORTRAN routine to evaluate the definite integral $\int_a^b f(x)dx$ of a function (integrand) of a real single precision floating-point argument x over the interval $a \leq x \leq b$
ANL D252S	DDFSUB	K. Paciorek	360 FORTRAN routine to perform one double precision integration step with step size $h \leq H$ for a system of N first order ordinary differential equations of the form $y_i' = f_i(x, y_1, \ldots, y_n)$, $i=1,\ldots,n$
ANL D253S	DDFSYS	K. Paciorek	360 FORTRAN routine to provide the input/output and control needed to perform a double precision integration of a system of first order ordinary differential equations using the subroutine ANL D252S, DDFSUB
ANL D254	DEGEAR	N. W. Clark and C. W. Gear	3600 FORTRAN routine for the numerical integration of ordinary differential equations with initial value boundary conditions
ANL E208S		K. Paciorek	Arbitrary Functional Fit for the 360 (least squares)
ANL E212S		J. Cohen	Evaluation of an arbitrary function for the 360 (least squares)
ANL E251	FITAPLOT	R. Odwazny	A low order least squares polynomial fit with plotting for the 3600
ANL F153	BORDER	B. Garbow	3600 FORTRAN routine for matrix inversion by bordering
ANL F105	MATEQ, UNIQUE	B. Garbow	3600 FORTRAN routine for the generalized solution of matrix equations
ANL F350	HYMAN	B. Garbow	3600 FORTRAN routine for determinant evaluation by Hyman's method

ANL F452	CHOLLU, CHOLEQ	B. Garbow	3600 FORTRAN routine for the symmetric decomposition of positive definite band matrices
ANL G551	RANNRM	D. Jordan	3600 routine to produce random numbers with normal (Gaussian) distribution with unit variance and zero mean
ANL J952S	YØLYPLØT	C. Chamot	360 FORTRAN routine to generate a CALCOMP tape for plotting a labelled graph of Y vs. X or $\log_{10}$ Y vs. X, given sets of values (X,Y) and plotting specifications
ANL J953	CDCIB	N. W. Clark	3600 routine to round and convert appropriately from CDC 3600 word format to IBM 360 word format
ANL J954	CDCIBW	N. W. Clark	3600 routine to pack, block and write binary tape records in a form acceptable for input to the IBM 360
ANL M250S	SMALLIST	R. Tannura	360 routine to decrease the size of IBM OS/360 assembler language listings to fit on 11-3/4 x 8-1/2" paper for submission to the AMD Program Library
ANL N251S	ABEND	G. Duffy	360 routine for the abnormal termination dump call from FORTRAN IV
ANL Q052S	CLOCK	G. Duffy	360 routine for the value of clock upon call from FORTRAN IV
ANL Q053S	COPYAGO	G. Duffy	360 routine to copy a load module from tape to disk and execute it
ANL Z013S		J. Herman	Variable metric minimization for the 360

Abstracts of Computing Center Newsletters

A new series of newsletters are being published irregularly and supersede the former 3600 Newsletter, whose last issue was number 34, dated June 14, 1966.

The aim of the new newsletters is to carry current information of interest to users of AMD computer services about both the CONTROL DATA 3600 and IBM 360 Systems as well as related areas.

Computing Center Newsletter No. 1 September 1, 1966

Updated release of 3600 SCOPE Operating System, ANL SYS 10-16.

SCOPE/SATCOPS II
FORTRAN 5.2
COMPASS Modifications
3600 FORTRAN Library Modifications
ALGOL 1.3
SNAP Modifications

Programming Systems Consulting.

580 Calcomp Plotting Package.

Use of 026 Key-punched FORTRAN Decks on S/360.

Interpreting S/360 Object Decks.

S/360 Model 50 Operating Highlights.

Hardware and Software Bug Reporting.

3600 FORTRAN 5.2 Diagnostic List.

Computing Center Newsletter No. 2 December, 1966

OS/360 (Release 7) Announcements.

3600 SCOPE System, ANL SYS 10-16A.

Modified Calcomp Packages.

New Computer Charges.

AMD Program Library Catalog.

Computing Center Newsletter No. 3 May, 1967

OS/360 (Release 11) Announcements.

MFT-Option II
Password Protection
FORTRAN IV (G) Compiler

Improved System 360 Documentation.

3600 SCOPE System, ANL SYS 10-17.

SCOPE 6.2
COMPASS 5.2
FORTRAN 5.3

DD80 Film Output from S/360 Jobs.

3600 FORTRAN to 360 FORTRAN Conversion.

Notes on Calcomp Turnaround.

OS/360 Course Announcement.

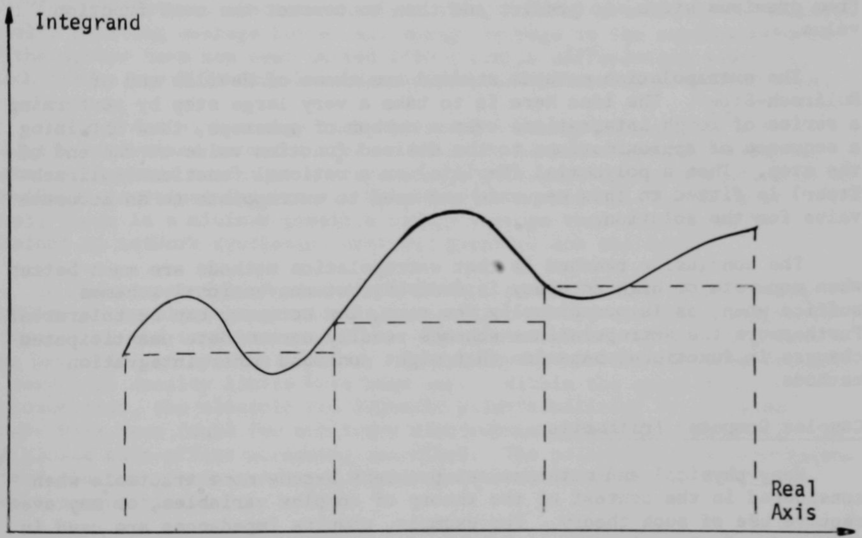
OS/360 Programming Systems Index.

NUMERICAL AND MATHEMATICAL RESEARCH

Real Numerical Quadrature Using Contours in the Complex Plane

A fundamental problem solved in a digital computer is to replace an integral (which may be thought of as the area under the integrand curve) with a finite sum which approximates it. Thus the basic definition of the integral is used in its calculation. Limitations of time and hence of cost imply that one should not use too many terms in the estimate. If the function being integrated oscillates rapidly, a large number of terms may be required to get reasonable accuracy.

Faced with this conflict, recourse may be made to complex variable theory, which allows one to calculate an integral along a curved path in the complex number plane instead of along a straight line segment on the real axis. By clever use of Hilbert transforms and by judicious choice of a function of a complex variable one may sometimes succeed in the calculation by using only a small number of values of the chosen "smooth" function at points of a curve in the complex plane.



The diagram illustrates that in the original problem many small rectangular areas may need to be summed to give a good approximation to an integral (or area). A visual description of the simplifying calculation would unfortunately require a four-dimensional picture.

Numerical Integration of Ordinary Differential Equations

An extensive and illuminating comparative study of various numerical methods for integrating ordinary differential equations has now been completed. While the older techniques used for comparison in the study are quite predictable in their behavior, the newer ones, based on extrapolation procedures, are at present most effectively judged by their empirical performance on a number of representative problems. The test problems used included the negative exponential problem, solution of Euler's equations of motion for rigid bodies in three dimensions, solution of Bessel's equation, and solution of the restricted three-body problem.

The methods used for comparison are those known as Runge-Kutta and Adams-Moulton. Runge-Kutta is a one-step procedure, utilizing only known and estimated information about the solution function and its derivative within the current integration step. Various approximations to the derivative are judiciously combined to give a high degree of accuracy for the increment of the solution across one step.

Multistep methods such as Adams-Moulton, on the other hand, make use of accumulated information about the solution and its derivative, obtained from previous steps, to predict and then to correct the next function value.

The extrapolation methods studied are those of Neville and of Bulirsch-Stoer. The idea here is to take a very large step by performing a series of rough integrations over a number of substeps, thus obtaining a sequence of approximations to the desired function value at the end of the step. Then a polynomial (Neville) or a rational function (Bulirsch-Stoer) is fitted to this sequence and used to extrapolate to an accurate value for the solution.

The conclusion reached is that extrapolation methods are much better when moderate or high accuracy is desired, but conventional schemes suffice when, as is occasionally the case, low accuracy can be tolerated. Furthermore the extrapolations schemes readily accommodate unanticipated changes in functional behavior that might confound other integration methods.

Complex Computer Arithmetic

Many physical and mathematical problems become more tractable when considered in the context of the theory of complex variables, or may even require use of such theory. For example, complex impedances are used in the study of electrical networks, the probability density in wave mechanics is related to the square modulus of the complex wave function, and polynomials often have complex roots even though all their coefficients are real.

On the other hand, actual computation using complex arithmetic has heretofore been avoided in computer solutions because a penalty factor varying between two and four or more must be paid over real arithmetic. Certain algorithms employing complex arithmetic, however, may not only be intrinsically simpler but also more reliable.

Two such algorithms — one for numerical differentiation and interpolation, the other for finding those zeros of a given analytic function which lie within a prescribed region of the complex plane — have recently been investigated. It was found that with complex arithmetic the roundoff error in numerical differentiation can be simply controlled and that zeros can be determined quite reliably. Furthermore, error estimation and iterative improvement of solutions may be easier.

A long-range possibility is that computer design include facilities — parallel processors, for example — that would reduce the present penalties associated with programmed complex arithmetic enough to make it competitive (where appropriate) with real arithmetic.

Electromagnetic Energy and Forces

For a loss-free electromagnetic system, several previously established results relating average forces and energy storage to the surface behavior of the system have now been united into a single differential equation, which treats the Boltzmann-Ehrenfest adiabatic theorem as a special case.

For systems with energy loss, forces and energy storage are not uniquely determined from the surface behavior alone. Thus, for example, there corresponds no unique average energy storage, to the excitation of a specified electrical impedance. However, for a rational impedance at least, there is a minimum possible energy storage that can always be attained by network synthesis, provided gyrators are employed.

In the assessment of plasma containment possibilities of particular high-frequency electromagnetic field configurations, the electromagnetic interactions and translational force associated with a sphere of plasma have been utilized by some workers. Invariably either low electron density or very high density limits have been used. Within the quasi-static approximation, the electric and magnetic polarizabilities of a plasma sphere have been found for arbitrary electron densities and the details of the plasma skin-effect screening described. The polarizability expressions extend the containment work and Slater perturbation theory to arbitrary electron densities.

Quantum Logic

The quantum logic approach to the foundations of quantum physics proposes an axiomatic structure for the collection E of "events" and the collection S of "states" of a physical system. Although the axioms are motivated by heuristic arguments about phenomenological experience, the resulting mathematical theory fails to provide mathematical constructs corresponding to several significant physical concepts, for example the concept of conditional probability. In conventional probability theory (where E possesses the structure of a Boolean algebra), the introduction of the mathematical construct corresponding to conditional probability is one of the elementary aspects of the theory. However, in quantum physics (where E possesses at most the structure of an orthomodular lattice, that is, the distributive law of Boolean algebra fails to be valid), the introduction of a mathematical construct corresponding to conditional probability is related to the quantum theory of measurements, the most controversial part of quantum physics from both a physical and philosophical point of view.

The purpose of this study has been to develop an extended axiomatic structure for the quantum logic approach which includes a mathematical construct corresponding to conditional probabilities.

A basic result of this study has been the recognition that the appropriate mathematical tools for the investigation of conditional probabilities are Baer *-semigroups. This phenomenologically motivated result is useful since there is a remarkable connection between the two abstract mathematical theories of orthomodular lattices and of Baer *-semigroups. Utilizing this connection it has been possible to reformulate mathematically significant but phenomenologically uninterpretable properties of the orthomodular lattice E as properties of a Baer *-semigroup which are both mathematically significant and phenomenologically interpretable.

Generating Functions for the Exact Solution of the Transport Equation

Generating functions have been used as analytic tools for the transformation of the integrodifferential transport equations to partial differential equations. The transformations are constructed so that their inverses are known. Therefore, the problem of solving the integrodifferential equations is reduced to the more familiar problem of solving partial differential equations of hyperbolic type. In the first part of the study the general method has been introduced in detail for slab geometry. The general solution has been given in analytic form, and the one-to-one correspondence with Case's method of elementary solutions demonstrated. The results were then extended to slab geometry without axial symmetry.

The second part extends the method to the general time-dependent, anisotropic case for slab geometry, while later work treats stationary and time-dependent problems in one and three space-dimensions by the method of characteristics, and includes numerical results.

Characterization of Criticality

There are several different ways in which criticality may be defined for a multiplicative transport process: in terms of the extinction probability, the limiting behavior of the mean number of particles at time t, or the behavior of the solution of the time-independent transport equation. It has now been proved that for a large class of processes involving particle multiplication on a line these criteria are all equivalent.

Error Analysis for Numerical Integration

Although a wide variety of numerical methods for the solution of ordinary differential equations and the computation of integrals have been developed, a thorough error analysis of such methods still reveals that there remain many complicated, unsolved problems. In order to avoid numerical calculations based only on the hope that the results will be accurate enough, much needs to be done for a proper treatment of such procedures.

New error bounds are being worked out for common quadrature rules, with emphasis on easy application to given problems. Especially useful are bounds not involving large derivatives.

The error of a one-step-method for ordinary differential equations can be reduced to a sum of errors of quadrature rules, thus leading to derivation of new, effective error estimates. This has been partly carried out already but further research will be necessary. Computer programs written for the CONTROL DATA 3600 support and confirm the above conclusions.

Natural Classification of Data

A continuing study is being made of natural classification schemes. The basis of such classifications of data is taken as economy or a possibility of economy in storage of independent samples of the data. Thus a natural classification amounts to a possibility of an encoding or compression of the data. Economy in storage without loss of information amounts to an overestimate of the entropy of the data. One of the ways of making an overestimate of the entropy is to classify the data. The classification with the lowest overestimate is the natural classification. A complete hierarchical tree of classification corresponds to a complete encoding (and an order or method of encoding) whereas a simple division into classes corresponds to a partial encoding. A level of classification useful for a particular purpose corresponds to an encoding for that purpose and the remaining entropy is noise for that purpose. Thus a purpose for the data may suggest one or a few among the many ways of dividing data into classes.

Smoothing Empirical Data

A paper concerning minimization criteria for smoothing empirical data is being put in final form. Consider a curve to lie "near" an empirical curve $k(x)$ if at every point x the two curves differ by less than the expected error of the empirical curve at x. The "smoothest" curve lying "near" $k(x)$ is taken as the function $y(x)$ which minimizes the integral

$$\int_{\alpha}^{\beta} f(x,k(x),y(x),y'(x),y''(x))dx$$

for some suitable function f. The paper concerns criteria for choosing appropriate integrands f.

Parabolic Partial Differential Equations

Varga has shown how certain rational approximations to e^{-x} on the semi-infinite interval $[0,\infty)$ lead to stable implicit methods for solving parabolic partial differential equations. In a continuation of this work, and in collaboration with Professor Varga, near minimax approximations to e^{-x} of the form $[1 + P_{n-1}(x)]/Q_n(x)$, where P and Q are polynomials, have been generated for $n=1,\ldots,14$.

Equilibrium States in Quantum Statistical Mechanics

An axiomatic C*-algebraic approach to the statistical mechanics of infinitely many particles has been proposed by Haag, Kastler, Ruelle, and others. The general features of the equilibrium states of quantum statistical mechanics at finite temperatures have been discussed by Haag, Hugenholtz, and Winnick. A C*-algebra A consisting of random variables or observables is constructed. A state of the physical system is identified with a positive normalized linear functional on this C*-algebra, the expectation value functional for the state. Time-evolution is described by a one-parameter group $t \to \alpha_t$, of automorphisms of A. The main mathematical tool of Haag, Hugenholtz, and Winnick, is a *-subalgebra A_α of "analytic elements" of A. A mapping j_β (formally, $j_\beta = \alpha_{\frac{i\beta}{2}}$) is utilized to give an algebraic formulation of the Kubo-Martin-Schwinger boundary condition for a state ω. A just completed paper (with Professor Daniel Kastler, University of Aix-Marseille, France) (1) fixes some points of mathematical rigor involved in the introduction of $\tilde{A}_\alpha$ and j_β; (2) clarifies the role of the α-invariance of ω; (3) utilizes the notion of quasi-unitary algebras as developed by Dixmier to unify the formalism; and (4) presents a physically significant interpretation of the Pukansky-Dixmier condition for the type of the associated von Neumann algebra.

Writing Projects

The two chapters, "One-Dimensional Diffusion Theory," by M. K. Butler and J. M. Cook, and "Mathematical Foundations," by J. M. Cook, I and VIII respectively of the book "Computing Methods in Reactor Physics" (Gordon and Breach) are now scheduled to appear early in 1968. Harold Greenspan is an editor of this book.

Work by J. E. Moyal and P. J. Brockwell is continuing on the book "Stochastic Transport Theory."

A chapter entitled "The Numerical Solution of Polynomial Equations and the Resultant Procedures," by E. H. Bareiss, is part of the new book "Mathematical Methods for Digital Computers, Vol. II," Ralston and Wilf, Editors (John Wiley, 1967).

COMPUTER UTILIZATION IN DIVISIONAL RESEARCH

The Argonne Reactor Computation System, ARC

The implementation of the first group of ARC program modules — reactor computation units that operate under the direction of a central operating system in a unified manner — is well under way. Once specified, these modules are written and debugged independently of one another. Each module serves as a programming "black box," and is defined externally in terms of files of input data required by the module and files of information produced by the module. Each such file of information is called a data set or a data module.

The program modules are designed so that several modules may be concatenated to form a complete program; a program thus formed is called a program module path. The prime criterion in module specification has been to minimize the time and cost of programming development. In practice, this has meant standardization to allow all paths to use the same modules for input preparation, processing of library data, and output editing. Once the initial library of program modules is completed, an even greater saving in development time is anticipated, since future modules may be written to form new paths that make use of proved modules already in the library.

The initial set of 16 modules constitutes four ARC paths. The first two paths provide one-dimensional diffusion theory and transport theory calculations, respectively. Experiences to date in implementing the ARC system have demonstrated the feasibility of the ARC concept of program modularity, but it has become apparent that the importance of two points was initially underestimated. These were the need to freeze the structure of the data sets involved in inter-module communication, and to schedule the order in which the modules constituting a path are to be completed.

While accomplishing the desired decrease in programming effort, modularization produces relatively inefficient paths: that is, a path comprised of several independent modules is in general larger, and executes more slowly, than would a comparable code that had been written as a self-contained, free-standing program. (The size factor is of minor importance since the modules may be overlaid in the computer memory.) The time factor must simply be accepted as a concomitant to modularization. A path of sufficient importance, however, may be optimized to reduce its execution time; in the limit this would be a reprogramming of the path to form a single module to be added to the library as a new, one-module path.

The ARC project has represented one of the more ambitious uses of the operating system software (OS/360) supplied with the Applied Mathematics Division's new IBM System/360 computers. The extreme flexibility of the OS/360 system, while providing many useful and necessary facilities, requires that the user provide a great amount of information to the system. The quantity of this information, together with the varied and complex formats in which it must be submitted, requires a great deal of programmer learning time; it also increases the possibility of making input errors. For these reasons the initial effort will be to provide production paths that look like stand-alone programs in order to minimize the complexity of the OS/360 cards required. Studies are being made as to the possibility of writing an interface system of some sort to act as a buffer between the user and OS/360.

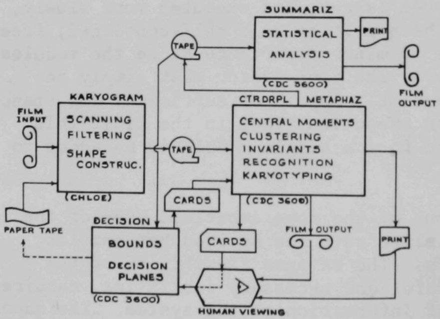
Perturbation Collapse in an Infinite Ocean

A flexible computer program has been written to solve the hydrodynamic equations describing the propagation of an oceanic perturbation, taking into account density variation, heat conduction, and viscosity. The initial perturbation is treated as the mixing of a small quantity of fluid at the center of a large rectangle whose sides are fictitious lines in an infinite two-dimensional ocean of fluid initially having a constant density gradient. The mixed fluid is released at time t=0 and then begins to collapse, spreading out to seek its own level. The program uses a two-dimensional, finite difference-type of algorithm in which boundary conditions are handled by extrapolation of analytic approximations to the solution at the boundary. It should now be possible to study the collapse of a density perturbation in a variety of cases which are of oceanographic interest.

The program output is in the form of tables of numerical values and 35mm film images produced at intervals during the computation. The film images are "snapshots" depicting constant pressure lines, constant density lines, and constant stream function lines at a given moment in time. These films give a total picture, easily evaluated by a human being, of what is happening in the system. Particularly interesting are the pictures showing the generation of internal waves in the stratified fluid as the mixed fluid collapses.

Biological Image Processing

A system of computer programs (using the CHLOE film scanner and CONTROL DATA 3600 computer) for the automatic analysis of metaphase chromosome images has been in operation for about one year. The present state of development of this system is such that it is necessary to process rather large amounts of data through it in order to measure its performance and pinpoint components needing improvement. A set of 835 chromosome spread images from a species of marmoset have now been run through the complete process; the results of this test are still being studied.



Block Diagram of System for Chromosome Data Analysis

Parts of this same system have also been used to investigate the automatic processing of bone autoradiographs and to study the relative mobility of malignant and non-malignant cells by analyzing time-lapse photographs, the second in cooperation with G. Barski of the Institut Gustave Roussy in Villejuif (France).

Automatic Theorem Proving

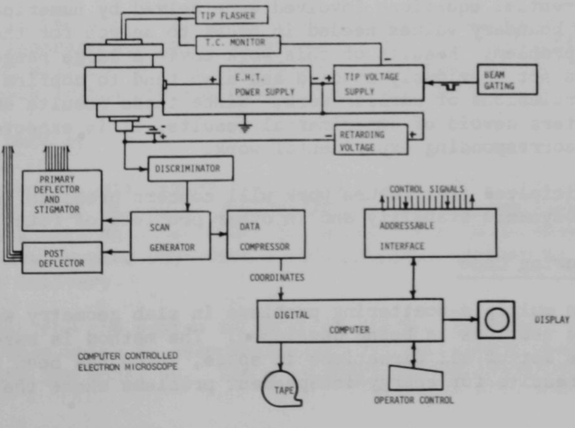
A new technique, demodulation, for substantially reducing redundancy in the search for proofs of theorems has been developed, tested, and implemented on the CONTROL DATA 3600 computer. Resulting economies in machine time and memory space have materially enlarged the realm of applicability of automatic theorem-proving procedures.

Machine-oriented rules of inference for that formal axiomatic system called the first-order predicate calculus with equality have been formulated, and a number of relevant metatheorems have been proved. An attempt is under way to prove the remaining lemmas required for a rigorous completeness proof. Preliminary studies are in progress concerning the problems of an efficient digital computer implementation of the new inference rules.

Electron Optics

Some minor improvements have been made in the system of programs developed for calculating the first- and third-order properties of axially symmetric electron lenses. In particular, the equipotential surface profiles for producing the required potential distribution on the lens axis can now be output in visual form via the Cathode Ray Tube film recorder on the CDC 3600 computer system. Using the improved programs, it has been found that accelerating lenses which are asymmetric along the z-axis can produce smaller spot sizes than previously used lenses symmetric around the central plane. Also, an asymmetric lens can be made less convergent, so that higher accelerating voltages can be used without bringing the beam to a focus inside the lens.

Further advances in electronic microscopy will require that microscopes be made easier to use and that better methods be found for using the information produced by these instruments. To implement these ideas, a scanning microscope is being designed to operate under the control of a digital computer; the same computer also stores image information from the microscope and executes analysis programs to aid in interpretation of the data. A machine of this type is a proper scientific tool capable of making quantitative measurements and is not simply a device for producing pictures.



COMPUTER CONTROLLED ELECTRON MICROSCOPE

Reactor Safety

In order to estimate the accidental damage potential of a proposed reactor, the reactor physicist studies the maximum credible accident of an idealized system. The major effort of these studies is devoted toward understanding the initiating circumstances. However, it is also necessary to calculate the reactivity reduction due to the explosive disassembly of a supercritical reactor. Work is in progress to add such calculations to a new quasi-static reactor kinetics code, QX1, which is being developed by the Reactor Physics Division. The reactor materials are assumed to behave like a non-viscous, compressible fluid, and the governing partial differential equations are solved by a finite difference method which smears out any shocks that may develop.

Study of Labelled Mitosis Curves

On the basis of a model for cell growth in which the life-cycle of a cell is divided into four phases with independently distributed time durations, a mathematical study is being made of radioactively labelled mitosis curves used to estimate the mean duration of each phase. For arbitrary probability densities of the phase durations, an analytic expression can be derived for the labelled mitosis curve. For computational purposes, the history of the cell population can also be simulated using the assumed lifetime densities in order to generate the labelled mitosis curve. Using these techniques it is planned to study the effect of statistical fluctuations on the labelled mitosis curve and to study how it can best be used to estimate the mean phase durations.

Viscous Fluid Studies

In the study of viscous, incompressible fluids, it is necessary to know when steady laminar motion becomes unstable. Work has been completed on a theoretical study of the stability of the spiral flow of viscous fluid confined between two concentric, rotating, circular cylinders with a pressure gradient acting along their common axes. Linear stability theory is used and asymptotic solutions have been derived for the governing sixth-order linear ordinary differential equation.

The differential equations involved were solved by numerical integration to produce the boundary values needed in order to search for the characteristic values of the problem. Results of this work cover a large range of the relevant flow parameters not previously studied and also tend to confirm the limited theoretical conclusions of earlier work. Since these results embrace a range of flow parameters devoid of experimental results, it is expected that they will stimulate the corresponding experimental work.

It is anticipated that future work will concern problems in the nonlinear theory of hydrodynamic stability and in other problems of rotating fluid systems.

Multiple Scattering Code

A code for multiple-scattering problems in slab geometry with energy-dependent cross sections is being developed. The method is based on a discretization of the set of all directions in space, which has been found to give very accurate results for energy-independent problems where the exact solution is known.

COMPUTER ENGINEERING RESEARCH AND DEVELOPMENT

Film Measuring Systems

Nature speaks to man through the tools of science in many ways but almost never in a form suitable for immediate processing by a digital computer. The smallest particles of matter are observed only with the aid of great particle accelerators since the very small can be observed only with the aid of particle probes of great energy. The events observed are recorded by the hundreds of thousands on ordinary photographic film, usually with four views to permit a three-dimensional reconstruction of what happened.

To get the numbers to put into a digital computer for the purpose of calculating the three-dimensional coordinates of the particle path from three planar views, and after this to find the equation of a helix that fits the path, requires elaborate measuring techniques. Many methods have been used, some involving extensive measurement by hand and others requiring very elaborate measuring devices.

POLLY I is a highly automatic cathode ray tube film scanning and measuring device which nevertheless permits operator intervention at strategic points where the controlling digital computer surrenders to the superior power of the human operator. The customary need for balance between cost and performance in engineering design has governed the development of POLLY I, which was built as a prototype device in the Applied Mathematics Division.

The precision of POLLY I is as good as that of conventional manual measuring tables. Indeed, the reliability and the possibility of statistically averaging errors may make POLLY superior in accuracy to manual methods.

A production version, POLLY II, currently being constructed in the High Energy Physics Division, uses a more sophisticated operator's position, involving a true optical display capability of the frame currently in the measuring system gate. A Scientific Data Systems Sigma 7 Computer is to be the control computer for this second system.

Interest in the POLLY design by scientists from European as well as United States laboratories makes it probable that modified copies will be widely used and will contribute substantially to breaking through what has been a bottleneck in the processing of high energy physics data.

Remote Access Data System

A Remote Access Data System (RADS) has passed its initial design stage and is entering early phases of implementation. Its message-switching computer (MSC) is a Data Machines 620-I to be delivered in December of this year. The IBM 2701 Data Adapter Unit with a parallel data adapter is scheduled for early November delivery.

Programming for the system is about to start. Version I will be in three parts: that which is associated with 1) the remote station, 2) the MSC, and 3) the IBM Model 50. The programming in the Model 50 occurs as modifications and additions to the ASP (Attached Support Processor) programming system. Version I will be written in a straightforward manner, with the prime use intended to be batch processing. Data compression techniques will not be included. Data input from the remote station will be in a card format (eighty columns per record) for each 20-record block of transmitted data. Messages or jobs can then be composed of one or more blocks of data. Input records will contain card images that contain the necessary control cards for the ASP and 360 programming systems.

The remote station, now under construction and evaluation, will have a Data Machines 620-I as a control computer, plus a card reader (NCR) and a line printer (POTTER). Two of its major elements, the computer and the card reader, are to be delivered in the summer of 1967, and delivery of the line printer is scheduled for November. The card reader electronics and card reader controller are being completed and tested. Transceivers which will be used to transfer data over common telephone lines at a 5000-bit-per-second rate have been under test for the last year. Recent error rates are one error in 100,000 records, for records of length 2048 bits. The final transceivers and controllers are under construction; when these are completed the remote station computer will be used both to transmit and to receive, in the further checking of the error rate over telephone lines. A controller for a Kennedy incremental magnetic tape is being designed. This will allow faster entry of both programs and data, and demonstrates the flexibility of a low cost IBM-compatible tape unit for low speed data gathering.

There will be no translation of codes in the Model 50 or the MSC. All device-dependent coding will initially be done in the remote station. Future versions of the system will take advantage of data compression techniques and make use of the high-speed paper tape equipment on the MSC for systems use. (See also under COMPUTER SYSTEMS AND LANGUAGES, IBM System 360 Development Project A.)

Computer-Controlled Diffraction Equipment

The ARCADE (ARgonne Computer Aided Diffraction Equipment) system, an on-line computer control system for directing and performing experiments in neutron or X-ray crystallography, is now being used successfully in control and data collection experiments using the full circle goniostat (crystal positioner) at Argonne's CP-5 reactor. It is also ready for use with a heavy duty diffractometer and cryo-orienter.

The goals of the ARCADE system are: 1) to eliminate as far as possible the hardware buffers, scalers, etc., that comprise present day semi-automatic equipment, 2) to produce an adaptable interface to allow necessary future expansion at small incremental costs, 3) to develop a standard monitor control program usable by the experimenter in a straightforward conversational mode. This direct communication with the experiment by simple typewriter commands is necessary since the growth of the system and the future needs of the experimenter are largely unpredictable.

The system is supplied with a large array of utility routines, an extensive arithmetic subroutine library, and a Real Time Monitor (RTM). Basically, the Real Time Monitor: 1) handles the loading from the disk of programs called from the keyboard; 2) establishes the transfer vector table, interrupt transfer vectors, and all disk communication; 3) directly controls the keyboard/printer communication interrupts; and 4) handles linkages of programs that are greater than one core (storage) load in size.

A large array of user programs for the ARCADE control system have been developed. Basic programs insert various constants, such as monitor count and chart recorder scale factors, and perform positioning functions of the motors during initial setup of the experiments. A least-squares program calculates lattice and instrument constants and their probable errors based on intensity information obtained from searching predefined diffraction peaks.

Using least-squares-determined constants, the data collection programs generate d-spacings and instrument angles under various options. The system then performs the automatic step-scan of peaks and collects the data to be used in further analysis programs, e.g., background, peak integrated intensity, number of steps, orientation. The measurement of standard reflections may be automatically interspersed with data collection and intensity comparison, and crystal reorientation can be selected by an experimenter option. Other programs are available for creating data files, specifying lists of reflections to be measured (either for peak-seek programs or standard measurement), describing crystal parameters, and so forth. Each is intended to allow flexible communication between the experimenter and his equipment when necessary, but also to provide a means of completely automating the procedures when appropriate.

The hardware interface was constructed primarily of integrated circuit logic and includes program-selectable prescalers for both the fission monitor and detector, the variable motor speed control (including acceleration and deceleration), a real-time clock, and hardware that is pertinent to the individual needs of the experimenters.

Opto-electronic Information Storage

A research project to determine the feasibility of storing binary information on photographic plates utilizing holographic* techniques is currently in progress. The ultimate goal is to store a 64x64-bit (binary digit) array of information in a holograph 2mm on a side. A 64x64 array of such holographs will be placed on an emulsion-covered glass plate, thus yielding a total information storage exceeding $16\text{x}10^6$ bits per plate. Since the process of storing information on the plate will consume a considerable amount of time by computer standards, the projected use is for read-only storage, e.g., assemblers, compilers, archival material. It is estimated that the writing and development will take approximately four hours.

Reading the stored information will be accomplished by utilizing a single detector array and switching the illuminating laser beam to the various holographs by means of a series of opto-electronic switches and bi-refringent crystals. With this technique it should be possible to select any of the holographs in the array in approximately four millionths of a second.

*A holograph is a photograph of a three-dimensional diffraction pattern.

Once a holograph has been selected and illuminated, its 4096 binary digits would be available in parallel. Utilization of the information can then be governed by conventional electronics.

An optical bench which eliminates the effects of building vibration has been constructed. Its relative vibration limitation is on the order of 1000 Angstrom units. This was accomplished by suspending a 3500-lb. granite plate on five air columns. These air columns are in turn suspended on a frame which has as its contact points only the areas of least vibration in the laboratory.

A number of holographs have been prepared, both of the reflected light type and of the direct transmission type. Efforts are currently being directed toward higher efficiency holographs of the desired storage density.

Holographic memories have great potential because they not only provide large storage capacity but also imply high reliability due to their redundancy.

Mössbauer-Effect Data Collection System

A small data collection system has been assembled at Argonne for use in conjunction with up to four Mössbauer-effect* experiments in the Physics Division. Initially three experiments have been interfaced to a small general-purpose computer (an SCC 650) through the direct-memory-access channel, with provisions for adding one more.

Each experiment utilizes a detector moved to and from a source so that the acceleration of the detector is linear. Each cycle of the detector is divided into 400 time-windows (channels). Data collection consists of adding the number of detector pulses associated with a particular time-window to the previously accumulated total for that same window. Total accumulations for a typical experiment require that double-precision storage be used. This results in 800 words of magnetic core storage per experiment. In addition, the computer is utilized in the "through accumulator mode" to control the display of the accumulated quantities for a selected experiment. This display is under program control, and the typewriter is used on an interrupt basis to select the experiment to be displayed and to display scale factors. The computer is also utilized for data manipulation in an off-line manner.

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*The Mössbauer effect is the absorption of energy by atomic nuclei, and its detection involves a phenomenon analogous to the familiar change in pitch of a train whistle as it approaches and recedes. Exploitation of this phenomenon, known as the Doppler effect, is the most frequently used technique for detecting incredibly precise energy changes occurring during absorption.

Initial results are very gratifying in the accumulation, control, and display areas. The control program gives the experimenter great flexibility by allowing him to enter various commands and parameters from the typewriter. Options include the initiation or deactivation of any of the experiments, display of any portion or all of any of the experiments at fifteen different scale factors, and binary-to-decimal conversion for output on either the typewriter or the paper tape punch.

Much of the effectiveness of this system is achieved by performing the additive functions for channels in the interface hardware. This feature permits a rapid and meaningful display under program control and even permits data accumulation when the computer is in a "halt" condition.

Automatic Fingerprint Classification

Research has continued in the area of primary fingerprint classification and identification. The classification phase of this work has been completed and was published in the Proceedings of the First National Symposium on Law Enforcement Science and Technology. By invitation of New York Congressman Scheuer, co-sponsor of a bill to create a National Institute of Criminal Justice, a display featuring this work was sent to Washington for an exhibit whose purpose was to dramatize the need for this type of research and to inform Congress on the desirability of creating such an institute.

Work is continuing on the second phase — identification. A program is being developed to extract ridge endings from a fingerprint pattern in the presence of noise. The approach taken is to trace the ridges by a system of tagging. If N ridges enter a smudged area and $(N\pm1)$ ridges exit the area, the program concludes that a ridge ending has occurred in the area. Using this ridge-ending information along with ridge-slope information, one should be able to specify a fingerprint to the extent that it may be located in a large fingerprint file.

Both phases have utilized Argonne's film-scanning system CHLOE to digitize pictorial fingerprint information.

Emulsion Track Counter

Development has reached the final stages on PAULETTE, a device designed to count automatically tracks made by atomic particles in a fine-grain emulsion. Instead of sharing a computer with several other engineering projects as it did heretofore, PAULETTE's scanner now has been interfaced to a dedicated PDP-9 computer. This is the final configuration for a multi-shift operation. A recent improvement is that the control program can now set multi-level discriminator trigger values. This was done to provide automatic compensation for varying background levels on the emulsion plate. Substantial effort has also been expended in the areas of automatic power-on and power-off interlocks to preclude equipment damage, and of initial parameter adjustment.

Laser Measuring Table

Feasibility studies of this device have determined that, although the principle of operation is perfectly valid, inherent instabilities render it impractical. The table, intended for use in measurement of bubble chamber photographs, uses a beam of coherent light from a helium-neon gas laser to replace the conventional wires connecting cross-hair indicator and shaft encoder. The feasibility question was whether the angle of a mirror on a rotatable shaft could be determined accurately enough. The original intent was to use the system in a closed loop feed-back mode so that the rotatable mirror always reflected the light from the laser out to the measuring cross-hairs and back to photo-detectors. Although the angular encoder utilized was inherently capable of determining the angle to the desired accuracy, the problem of repeatability was affected by both temperature and low amplitude noise, to the degree that the cost of the system could not be justified.

The system was also evaluated using the mirror in a constant angular velocity mode. It was intended that the time difference between the reflection directly back from the mirror and the reflection back from the cross-hairs would determine the angle. Again, this principle in theory is certainly valid. The results from this method, while better than those of the previous method, were still not gratifying enough to warrant continuation of the project.

APPLIED PROGRAMMING SECTION

In the course of the year, a reorganization of the groups in the Applied Programming Section has occurred. Heretofore the section organization paralleled the divisional structure of the Laboratory. The reorganization is based rather on functional demarcations and should allow problems to be better matched to the interests and abilities of group members. The four current groups in the section are: Theoretical Physics and Chemistry, Experimental Science, Reactor Theory and Development, and Engineering and Applied Systems. In addition, an Assignment and Review Board has been formed to coordinate initiation of new work and evaluate progress of work underway.

Theoretical Physics and Chemistry

A technique to calculate ballistic trajectories through a magnetic beam spectrometer composed of varying magnetic fields was implemented. In conjunction, programs for the fitting of magnetic fringe fields and for the calculation and statistical analysis of resolution functions were developed.

Through series and asymptotic expansions and rational function approximations, a variable representing a ratio of temperature characteristics in the Debye Specific Heat Function was determined.

A program was written to calculate the energy levels and corresponding wave functions of a nucleon (neutron or proton) bound in a spherically symmetric potential.

A further program was written to compute and plot the electron spin resonance (ESR) line shapes that correspond to those observed in compounds of the MH_2AO_4 type.

A compiler has been written in PL/I to translate equations representing chemical reactions and balance relations into FORTRAN for inclusion into subroutines called in the solution of partial differential equations arising in diffusion kinetics.

Experimental Science

Some crystallographic programs have been combined into an overlay system for operating upon diffraction data. These include a correction for Lorentz polarization and spherical absorption effects, least-square refinement, and a sorting of indices and Fourier summation. A triple product direct method has also been programmed.

Problems of a basically statistical nature included plume rise from smoke stacks and an analysis of EBR2 fuel pin swelling. Programmed as a Monte-Carlo calculation was the simulation of labeled mitosis curves. Further problems involved a statistical analysis of partially ordered defects in nonstoichiometric ionic crystals, and the calculation of metal-water reactions during a loss-of-coolant reactor accident.

In the management information area, programs written produced computer services reports for laboratory accounting, including actual and projected program costs.

Reactor Theory and Development

The implementation of the first group of ARC (Argonne Reactor Computation) program modules, as described in the previous report (ANL-7280) is well underway. Specifically, an initial set of 16 modules, which will constitute four ARC paths, is nearing completion. The experiences to date in implementing the ARC system have demonstrated the feasibility of the ARC concept of program modularity — that is, the possibility of writing a number of independent modules, each of which is defined externally in terms of the data sets required and the data sets produced, and of then concatenating these modules to form a path (i.e., a set of linked modules forming a program).

Other programming within the group provided for solution of problems in the theory of elastic vibrations and determination of models for the theory of radiation injury and recovery in self-renewing cell populations. Techniques required included inversion of finite Hankel transforms and solution of systems of differential and integro-differential equations.

Engineering and Applied Systems

Experimental control programs have been written on the IBM 1130 computer for the Neutron Diffractometer and on the ASI 210 for the 70-inch scattering chamber. A program for the 360 has been written to assemble programs written in 1130 Assembler Language.

A calibration system has been completed for the Bubble Chamber film measuring system POLLY I. A PDP-7 program measures the calibration grid, and a 3600 fitting program determines the actual calibration coefficients.

The Library system under development includes a program which accepts blocked data on magnetic tape, performs operations on entries such as editing and descriptor generation, and provides output again in blocked form on tape. A related program creates, updates, and lists the User Profile file.

The following programs have been completed by the Applied Programming Section in the past year:

B126 TEMPERATURE CORRECTION FOR BOMB CALORIMETRIC DATA

From resistance readings, this program calculates corresponding temperatures (in degrees centigrade) which reflect the effects of a specific thermometer, constant stirring, and heat exchange with environment.

B127 TEMPERATURE CORRECTION FOR BOMB CALORIMETRIC DATA

Same computations as B126, but utilizes the effects of a different thermometer.

B137 A MODIFICATION OF ANL-FLS, MET153 PROGRAM TO ACCOUNT FOR OVERLAPPED DATA

This modification of MET153, ANL-FLS, A FORTRAN Crystallographic Program, performs least-squares refinement of crystal structure parameters for a twinned single crystal and powder diffraction data.

B172 DEVELOPMENT OF FORMULAS FOR THE INVERSE OF THE ERROR FUNCTION

Formulas are given for computing the inverse of the error function to at least 18 significant decimal digits for all possible arguments up to 1-10**(-300) in magnitude.

A formula which yields erf(x) to at least 22 decimal places for abs(x) ≤ 2.5*PI(PI = 3.14···) is also developed.

B197 CORRELATING FUNCTIONS FOR DISSOLUTION OF URANIUM IN CADMIUM

Correlating functions for dissolution of uranium in cadmium are evaluated by correlation of mass transfer coefficients with various parameters of the system.

B207 VISCOSITY OF LIQUIDS

This program provides for the calculation of liquid viscosity from experimental data obtained on the attenuation of an oscillating (torsion pendulum) cup viscometer. The attenuation is expressed as the log decrement. Two different experimental arrangements can be handled: (1) that for an "open cup" viscometer, in which the top liquid surface is free and (2) that for a "closed cup" viscometer, in which both upper and lower surfaces of the liquid are in contact with the viscometer.

B209 ORSTAT, A FORTRAN PROGRAM FOR THE STATISTICAL ANALYSIS OF DIFFRACTION DATA

The program calculates the probability distributions of intensities of X-rays diffracted by crystal lattices. It performs Wilson averaging, statistical tests for symmetry elements, or the two calculations in sequence.

B219 POLYCRYSTALLINE NEUTRON-DIFFRACTION DATA - PROCESSING PROGRAM

The program processes the collected polycrystalline neutron count data by taking into consideration the required corrections for the absorption and Lorentz effects.

The optional output from this program is punched on cards and/or plotted using CALCOMP Magnetic Tape Plotting System #580.

B234 STATISTICAL ANALYSIS OF PARTIALLY ORDERED DEFECTS IN NONSTOICHIOMETRIC IONIC CRYSTALS

Nonstoichiometric crystals contain defects which, contrary to the common assumption of statistical analyses, are probably not randomly distributed over the eligible lattice positions. This present treatment assumes that defects of a particular kind (such as anion vacancies) repel each other from nearby sites; the number of sites a defect controls is then related to its position in a series of energy levels. The distribution and interaction energy functions arising from this model are substituted into a grand partition function for defects in a nonstoichiometric crystal.

B237 NEUTRON WAVELENGTH DETERMINATION

Determination of neutron wave length is made by a two-parameter linear least-squares fit.

B238 TABLES OF $AX + BX^2$

This program obtains a table of values of $AX + BX^2$ for X = 0[1]500, and given A, B.

B239 CALCULATION OF THE EXTENT OF METAL-WATER REACTION DURING THE HEATING OF A FUEL ROD IN FLOWING STEAM

This program computes the temperature of a fuel rod, the temperature of the rod cladding, the amount of rod cladding reacted with the steam, and the mole fraction of the steam as functions of time and axial position on the rod.

B240 STATISTICAL ANALYSIS OF AUTORADIOGRAPHY DATA

This is a four-part program calculating statistics such as means, variances, and tables of frequency or probability distributions.

B241 INDEX, A COMPUTER PROGRAM FOR INDEXING X-RAY DIFFRACTION POWDER PATTERNS

The program indexes the set of 2θ reflections, where θ is the Bragg angle as measured by a diffractometer from a powdered crystalline sample, on the basis of the cubic, hexagonal, tetragonal and orthorhombic systems. All lattice constants are calculated by an iterative least-squares procedure. The printed output includes the crystal system, the lattice constants and their standard deviations, the wavelengths used, observed and calculated $\sin\theta$ squared values, and the difference between these latter two.

B242 CRYSTALLOGRAPHIC DATA REDUCTION AND SCALING

This program accepts X-ray single crystal diffraction data and calculates the intensities for the film readings, corrected for Lp and spot shape effects. Then the program calculates the best possible intensities from the averaged values on different films and different layers.

The program is applicable primarily to the data obtained on film with Weissenberg and/or precession goniometers.

B243 INTEGRALS FOR PLASTIC STRESS AND STRAIN

This program will produce a table of integrals whose integrands are functions of EXP[(X*SQRT(1-X**2)-ARCSIN(X))/2*S**2], where S is input.

B246 SCATTERING OF WAVES BY OBSTACLES

A second-order differential equation in three independent variables is known to possess a closed form analytic solution subject to suitable boundary conditions. Solutions corresponding to three different boundary conditions are obtained by using finite differences, and these results are compared to the exact solutions to obtain the error estimate in the finite difference solution. Each of these solutions is obtained for three different grid sizes.

B248 DISTCOEF - METAL FLUX DISTRIBUTION STUDIES

This program computes and tabulates distribution coefficients and molar composition for metal-salt mixtures from the weight percent of metal found in each phase. Up to 10 components can be handled.

B249 VARIABLE METRIC MINIMIZATION

This is a general routine to determine local minima of positive differentiable functions. In the process an accurate error matrix is built up. Options include imposition of linear constraints upon the variables.

B251 TEMPERATURE CORRECTION FOR BOMB CALORIMETRIC DATA

From resistance readings, this program calculates corresponding temperatures (in degree centigrade) which reflect the effects of a specific thermometer, constant stirring, and heat exchange with environment.

B252 RESISTANCE TO TEMPERATURE CONVERSION

A Callendar equation is used to compute a table of resistances for a given thermometer at equal temperature intervals.

B253 FREE ENERGY OF MIXING

The program computes the free energy of mixing of a two-component system, by Lumsden's Method, from the composition of the miscibility envelope.

B254 PLOT INTENSITY DATA

This program reads the intensity data and the angle positions, and plots off-line these data vs. 2·THETA or sin(THETA/LAMBDA) values.

An option of subtracting the background, which may be read as the first set of data, is included.

B255 PLUTONIUM PILOT PLANT DATA ANALYSIS

This program performs data reduction calculations for a plutonium pilot plant.

B256 ESTIMATION OF TRIPLE PRODUCT

This program uses Triples formula for phase determination in centrosymmetric crystals with equal atoms and of monoclinic or higher symmetry. It may be used to obtain signs in the initial stage of phase determining procedures. Three-dimensional data is required.

B257 CALCULATION OF THERMODYNAMIC FUNCTIONS OF GASES

This program will produce a table of functions corresponding to Gibbs' Energy, Enthalpy, Entropy, Equilibrium Constant, and others which represent thermodynamic properties of an ideal gas.

B258 CALCULATION OF PHASE DIAGRAM

The program will determine the value T_e from the equation

$$RT_e \ \ell n\,((1 + x)/2) = RT_e \ \ell nx + D(T_m - T_e)/T_m + A(T_e \ \ell n(T_m/T_e) - T_m + T_e) + B(T_m - T_e)^{**}2 \ ,$$

where R, x, T_m, D, A, and B are input parameters.

B263 SOLUBILITY AND OXIDATION

This program determines the oxygen content of uncracked film and evaluates a function representing weight gain.

B264 GRAPHITE OXIDATION KINETICS

This program produces a table of successive convolution integrals which correspond to the quantity of atoms burned off in various layers of a piece of graphite.

C102 REPULSIVE SQUARE-WELL CALCULATIONS

The problem is to calculate the scattering of a particle (with energy related to k) by a spherical repulsive potential (with depth related to k_o and radius a).

C119 LEAST-SQUARES FIT TO TRIGONOMETRIC FUNCTIONS

This program finds best fit parameters for magnetic resonance data as a function of magnetic field orientation.

C143 PHONON SCATTERING BY VACANCIES

The program evaluates integrals of the product of a function of z involving exponentials and a specified function F(z, T, p), where p is a parameter set. The program may also be used to determine one of the parameters from the condition that the integral take on a specified value for a specified T.

C148 KINETIC ANALYSIS OF CONSECUTIVE IRREVERSIBLE SECOND-ORDER REACTIONS

A least-squares fitting procedure is used to find rate constants for two reactions.

C154 FOUR-PARAMETER SORTING OF BINARY DATA

Binary data contained on tape consist of events each divided into four parameters. Frequency distributions are found for specified parameters, given restrictions on the others. A total frequency distribution for all parameters is also produced.

C168 CALCULATION AND PLOTTING OF SIMULATED MAGNETIC RESONANCE SPECTRA OF CRYSTALS (OR SOLUTIONS)

A spectral function $F_k(x)$, consisting of the superposition of magnetic resonance lines of specified lineshape (either Gaussian or Lorentzian), along a magnetic field x, is generated and optionally plotted. The first three derivatives of $F_k(x)$ are also calculated.

C185 DEBYE SPECIFIC HEAT FUNCTION

For a given value of the specific heat of a solid, the ratio of the temperature characteristic for that solid to the absolute temperature is determined from the DEBYE specific heat function. The program is written in the form of a subroutine.

C189 DATA PLOTTING FOR FUEL REPROCESSING

Measurements of up to 200 parameters are given as a function of time. Specified parameters may be plotted with up to 4 curves on a graph.

C191 HIGH-ENERGY FISSION FRAGMENT ANALYSIS

The program reads a magnetic tape containing 48-bit words specifying 7 parameters for each event, and generates frequency distribution tables.

C193 PROFILE - CALCULATION OF RESOLUTION FUNCTIONS

Resolution functions are calculated, with the use of the optical expansion coefficients, over a large number of points in initial source space with the results presented as a histogram of the particular computed display coordinate.

C195 DETERMINATION OF FRINGE-FIELD MODELS

The variable metric method is employed to fit a non-linear least-squares function to obtain the parameters for a magnetic fringe-field model.

C197 PACKARD DATA TAPE ANALYSIS

A FORTRAN driver calls a COMPASS-coded subroutine REPACK which reads tapes from the MODEL 123 PACKARD system and analyzes them. Total frequency distributions are calculated.

C199 TRANSFORMATION OF C175 INPUT TAPES TO FIT MORE THAN ONE CONFIGURATION

This program generates an input tape (from data for several configurations) which may be used with the single configuration fitting programs C175 or C106 to fit parameters to levels from several configurations.

C201 ANL E212S - A GENERAL LEAST-SQUARES FITTING PROGRAM AND EVALUATOR FOR FUNCTIONS LINEAR IN THE COEFFICIENTS

This general program fits, in the least-squares sense, a set of observed values to a function which may be expressed as the sum of up to 41 terms where each term is the product of a fitting coefficient and specified functions of up to 10 independent variables. The program may also be used to evaluate such arbitrary functions.

C202 TSTPLT: ANALYSIS OF DELAYED COINCIDENCE EXPERIMENT

Convolution integrals together with specified moments are calculated and compared in determining the unknown lifetimes from measured data in delayed coincidence experiments.

C203 YOLYPLOT: PLOTTING ROUTINE FOR GRAPHS OF Y OR LOG Y VS. X

Given sets of values (X,Y) and plotting specifications, the subroutine generates a labelled CALCOMP graph of either Y vs. X or log Y vs. X.

C204 ANOMALOUS HEAT CAPACITY

Given x_o and d, the program evaluates the integral over (0,1) of a function $f(x,x_o,d,THETA/T)$ for various values of THETA/T.

H132 ASI 6020 TAPE-TO-CARD CONVERSION

This is a program for converting ASI 6020 paper tape to cards. All upper case characters are preceded by a SHIFT UP and followed by a SHIFT DOWN character on tape. A CARRIAGE RETURN character is an end-of-record code, signaling the end of the card image.

I108A THE RESPONSE OF GAMMA RAYS IN MATTER

The theoretical energy loss spectrum and other detector response parameters are calculated for various materials by the Monte Carlo method. These materials are (1) germanium, (2) silicon, (3) sodium-iodide, (4) cesium-iodide, and (5) Pilot "B". The program allows numerous source geometries of mono-energetic gamma rays varying in energy from 10 KEV. to 12 MEV. The detector shapes are (1) right circular cylinder and (2) parallelepiped.

I112 JOURNAL CHANGE PROGRAM

This program accepts cards containing journal change information and updates the journal file tape.

I121 CARD-TO-TAPE TRANSLATOR

This program reads BCD cards and outputs BCD card images onto magnetic tape. The character ordinarily interpreted as the end-of-file indicator is interpreted differently here.

P114 GRAPHICAL DATA REDUCTION ON THE ASI-2100 OR ASI-210

This FORTRAN callable subroutine written for the ASI-210 or ASI-2100 displays points on the DD16B oscilloscope. The program computes peak areas and subtracts areas of background drawn by the user with the oscilloscope attached light pen.

P141 CYLINDRICAL CAVITY FIELD COMPUTATIONS

The components of the electromagnetic field and the containment potentials in a resonant cylindrical cavity are computed for either the transverse-magnetic or the transverse-electric mode. Graphs of potentials vs. radial distance may also be obtained.

P142 FIFTEEN YEAR CLIMATOLOGICAL SUMMARY REPORT

This program prepares numerous tables from climatological data gathered by meteorologists at Argonne during the period from January, 1950 to December, 1964.

P143 MÖSSBAUER SPECTROSCOPY PROGRAMS

This is a set of programs to calculate Mössbauer spectra. There are three basic programs: UNIXTL, which calculates spectra for a single crystal source or absorber in an external magnetic field; LVSPHS, which calculates spectra for materials like Laves Phase alloys which are powders having internal magnetic fields fixed with respect to the crystal axes; and PDRHXT, which calculates spectra for randomly oriented powders in a fixed external field.

Later versions of UNIXTL and LVSPHS have been added; they calculate spectra for transitions of mixed multipolarity. These programs are called AUNIXT and ALVSPH.

P151 ATMOS I - A TWO-DIMENSIONAL MODEL OF THE ATMOSPHERE

This program retrieves information from a file created with the CDC 3600 SORT II system. The file contains card images arranged in sequence by key fields. The data reduction is accomplished through the use of Variables of Interest cards and a user-supplied data analysis subroutine.

P152 ANALYSIS OF WIND TURBULENCE

This program reduces and does spectral analyses of bi-vane wind data.

P158 INTEGER-PRESERVING GAUSSIAN ELIMINATION

An algorithm developed to permit integer-preserving elimination in systems of linear equations is implemented. Features of the algorithm include a) minimization of the magnitudes of the coefficients in the successive elimination steps and b) improvement in computational efficiency over ordinary Gaussian elimination.

P159 INPUT/OUTPUT SUBROUTINES

This report includes a series of eight separate input/output subroutines for the ASI-210 or ASI-2100 computers. All routines are FORTRAN-compatible and entry is accomplished via the CALL statement. The list includes

A. An IBM-523 card read-punch program.
B. A magnetic tape binary read/write program.
C. An alphanumeric typewriter input/output program.
D. A magnetic tape rewind program.
E. A typewriter integer input program.
F. A typewriter integer output program.
G. A line-printer integer output program.
H. A specialized line-printer integer output program.

P161 ENERGY LEVELS AND WAVE FUNCTIONS OF A BOUND NUCLEON

The energy levels and corresponding wave functions of a nucleon (neutron or proton) bound in a spherically symmetric potential are computed. The wave functions are solutions of the radial Schrödinger equation. Estimates for the energy levels (eigenvalues) must be supplied.

P162 CALCULATION OF A CALIBRATION FACTOR FOR A MULTICHANNEL ANALYZER

The calibration factor for a multichannel pulse-height analyzer is determined.

P163 CALCULATION OF Q-VALUES FOR NUCLEAR REACTIONS

This program calculates Q-values for nuclear reactions from the positions of peaks in a spectrum. At least one Q-value and the calibration factor for the multichannel analyzer must be known.

P164 DETERMINATION OF SCATTERING CROSS-SECTIONS FROM PULSE-HEIGHT SPECTRA

The differential cross-sections for elastic and inelastic scattering are determined as a function of scattering angle from an analysis of pulse-height spectra.

P165 TRANSFORMATION OF KINEMATIC QUANTITIES TO THE CENTER-OF-MASS SYSTEM

Various kinematic quantities are transformed (relativistically) from the laboratory system to the center-of-mass system.

P168 STRATIFICATION OF DEW POINT VARIABLES

A joint frequency distribution of dew point, temperature differential, wind speed, relative humidity and net radiation flux is prepared.

P169 PLOT CDC 3600 CALCOMP TAPES

CALCOMP output tapes generated on the CDC 3600 at 200 bits per inch (bpi) may be processed by plotters attached to the ASI-210 and ASI-2100 computers located in the Physics Building. The 200-bpi format is not compatible with the 580 Off-Line CALCOMP plotting system.

P170 CALCULATION OF CROSS-SECTIONS FROM RESONANCE PARAMETERS

This routine calculates neutron scattering cross-sections from resonance parameters using the Breit-Wigner Multiple-Level formula.

P171 PHYSICS SYSTEM 169 CONTROLS PROGRAMS

Two subroutines comprise a package to control beam shutter and scaler racks, and to set up the integrator interrupt fixed address to allow proper handling of interrupts.

P172 SINGLE-LEVEL PEAK HEIGHTS OF NEUTRON SCATTERING

This program calculates possible single-level peak heights of neutron scattering resonances in the Kev region.

P174 PLUME RISE

This program calculates correction multipliers to apply to least-squares regression equations for determining plume rise from stacks.

P175 PIE-PHOTOIONIZATION EFFICIENCY

PIE is a program to reduce photoionization experimental data to photoionization efficiencies and to plot these computed values versus wavelength.

P176 70-INCH SCATTERING CHAMBER CONTROL PROGRAMS

The scattering chamber contains four individually moving arms each of which carries a detector. The chamber also contains a target changer which can be loaded with up to eight targets. This set of subroutines provides for: forward or reverse azimuthal movement of a selected detector, inward or outward radial movement of a selected detector along the length of its arm, and selection of that target to be bombarded by the beam.

P177 2-D PACKARD TAPE-TO-CARD CONVERSION

This program will produce both punched-card output and printer output from punched paper tape.

Cards are punched in a format suitable for input to CANDY, an analysis program developed in the Physics Division.

P178 PHYSICS SYSTEM 169 CONTROLS PROGRAMS E.D.51,54

This subroutine with two entry points allows for transferral of data from scalers to ASI memory and for transmittal of frequency meter contents to ASI memory.

P179 INTERRUPT ROUTINES FOR ASI-210

Eight subroutines comprise a package to set up specific addresses for proper handling of interrupts.

R111 ACORN - AUTO-CORRELATION, CROSS-CORRELATION, POWER SPECTRUM

Data records of various sizes and formats containing information in 36-bit words on low density magnetic tapes are checked for errors and converted to 48-bit words on high density magnetic tape. Auto-correlation, cross-correlation, and noise-rejection routines are provided for computations on converted data. Various options are available to conserve tape-handling time and to allow maximum flexibility in treating large data samples.

R129 SHUTDOWN

An analytic expression for aftercooling power of a nuclear reactor has been programmed and applied to typical nuclear rocket shutdown schedules.

R144 STDY-3 (WAPD) - REACTOR THERMAL ANALYSIS

STDY-3 is a program for the thermal analysis of a pressurized water nuclear reactor during steady-state operation.

R156 FOIL COUNT CALCULATIONS

This program processes and plots weighted foil count data. The background and the counter corrections are also considered.

R158 HEX - EVALUATION OF HEXAGONAL FUEL ELEMENTS

This program smooths data from a fuel element whose cross-section is hexagonal.

R170 WIGL2 (WAPD) - SOLUTION OF SPACE-TIME DIFFUSION EQUATIONS

WIGL2 is a program for the solution of the one-dimensional, two-group, space-time diffusion equations accounting for temperature, xenon, and control feedback.

CHM193 EXTENSION OF PROGRAM 1518/CHM156

This program will obtain a table of a quadratic function AX + BX**2, where A and B are functions of input values.

PHY299 A GAMMA-RAY-SPECTRUM FITTING PROGRAM

A gamma-ray spectrum consisting of two experimental peaks, cosmic-ray background, and low-energy background is resolved into its components. The experimental peaks are fitted (in the least-squares sense) to given spectral shapes and the relative intensity of each peak is determined.

PHY310 POLARIS - DATA ANALYSIS FROM NEUTRON SCATTERING EXPERIMENTS

This PHYLIS system program analyzes data from neutron scattering experiments.

PHY312 COMBO - POLARIZATION AND DIFFERENTIAL CROSS SECTIONS FOR ELASTICALLY SCATTERED NEUTRONS

This is a PHYLIS system program wherein the polarization and differential cross section for neutrons elastically scattered from zero-spin nuclei are calculated by employing the R-matrix formalism.

02E6007 CALCULATION INVOLVING THE OUTPUT OF RE122

This program performs data reduction calculations using the output of RE122.

05E7003 POWER FUNCTION FIT TO ACTIVITY RETENTION DATA

A set of weighted points (t,y) is fitted to the form $y = x_1(t+x_2)^{-x_3}$ by the least-squares procedure.

10E7040 FLUORINE EFFICIENCY CALCULATION

This program determines fluorine efficiency from data obtained in a plutonium pilot plant.

12E7039 REDUCTION OF MÖSSBAUER DATA

This program is an extension of 2151/PHY303, Line Shape Fitting by Variable Metric Minimization. There exists an option to plot results on either the DD80 or CALCOMP 580.

14E7043 A FORTRAN CRYSTALLOGRAPHIC LEAST-SQUARES REFINEMENT PROGRAM

The program performs the least-squares refinement on crystal structure parameters based on X-ray or neutron diffraction measurements.

This program permits 1) the use of both isotropic and anisotropic temperature factors based on the individual atom selection, 2) the choice of scaling the change of the individual parameters varied, 3) the treatment of atoms in the special positions using the input cards, and 4) the correction of X-ray data for anomalous dispersion effects. The basis of this program is MET153.

16E7053 FLUORINATION RATE MODEL

The parameters involved in a relationship between the weight of PuF_4 and the rate of fluorination reaction are determined using a least-squares technique.

07R7020 CHOPPED - CALCULATION OF HYDRODYNAMIC PERFORMANCE BOILING WATER REACTOR CORES

Calculation of hydrodynamic characteristics of flow channels circulating a two-phase mixture of water.

10R7055 SNARG 1D - COMPOSITION CROSS SECTION OVERLAY TAPE

This program prints and punches the composition cross sections of SNARG 1D (R137) utilizing no more input data than a normal SNARG 1D run.

07S7010 A1130 - IBM 1130 OFF-LINE ASSEMBLY PROGRAM

The A1130 assembly program assembles programs written in IBM 1130 ASSEMBLER LANGUAGE off-line on the IBM 360/50 machine. A macro generator has been added to allow the user to define and use macro instructions.

09S7017 PAPER TAPE TO MAGNETIC TAPE CONVERSION

This program allows conversion of paper tape data to magnetic tape, for use as input to the CDC 3600 computer, with an associated printer listing. The program checks for illegal characters and short and long words; a tally of these errors is given on the printer listing, along with indications of where these errors occurred.

10S7021 CARD-TO-G.E. PAPER-TAPE CONVERSION

Conversion of punched card input to punched paper tape for use with the General Electric Computer Time-Sharing Service.

11S7034 MATCHING OF SECTIONS OF FLOOR OF HILBERT DOMAINS

This program represents a modification of P-130 wherein the three-dimensional rectangular grid is replaced by the two-dimensional surface of a tetrahedron.

12S7035 ASCII PAPER TAPE CONVERSION

Conversion of ASCII paper tape to magnetic tape or, optionally, to punched cards is provided. A printer listing is also obtained.

13S7048 SEL-810 PAPER TAPE CONVERSION

This program permits conversion of punched paper tape to punched cards or magnetic tape or conversion of cards or magnetic tape to punched paper tape.

01T6004 RESPONSE CORRECTION OF FLUORESCENCE EMISSION SPECTRA

Emission spectra are corrected for instrument response errors and plotted on the CALCOMP plotter. Also, various quantities characteristic of the spectra are computed.

02T7004 CALCULATION OF BINDING ENERGIES

A least-squares determination of parameters a_i, b_i, and c_i in the Wing-Fong Nuclidic Mass Equation is made.

07T7018 CALCULATION OF BINDING ENERGIES - Part II

This is a least-squares determination of the constants in the Wing-Fong Nuclidic Mass Equation.

10T7023 PLASTIC BEHAVIOR OF VANADIUM-BASE ALLOYS

Given a value of AO for the specimen, and E, P (stress, strain) data for the case of uniform plastic flow, the program determines values of K and N in S = K*D**N, where

S(OBS = (P/AO)*(1 + E) and D = LN(1 + E).

12T7025 DETERMINATION OF SLATER PARAMETERS

This is a modification of C175 to obtain matrix coefficients for up to 7 parameters from the Berkeley version of the MIT tape, and to incorporate appropriate coefficients for an additional parameter E0.

14T7028 INTEGRATION OF GAUSSIAN SPECTRAL DATA

Peaks of spectral absorption data are determined by least-squares fitting to sums of either Gaussian distributions or Lorentzian distributions or products of the two. Finally integrals for each peak are computed. This is an IBM System 360 version of the program C151.

15T7031 CALCULATION OF ELECTRONIC TRANSITION PROBABILITIES

The program calculates theoretical probabilities for electronic transitions between a ground state of an ionized atom and a large number of its excited states. Two different mechanisms for the transitions are considered, namely, electric dipole and magnetic dipole. Also included is an option to fit, by least squares, the results of the electric dipole calculation to various energy levels found in 1849/CHM177.

28T7069 CALCULATION OF LEVITATION FUNCTION

Evaluation of the levitation function by rational polynomial and Taylor series approximations is made.

30T7071 THEORETICAL WIDTH DISTRIBUTION FUNCTIONS

This program provides evaluation and plotting of four expressions involving Gamma functions and modified Bessel functions.

31T7072 AVERAGE PROPERTIES OF A SET OF RANDOM HERMITIAN MATRICES

Average properties of the eigenvectors of a set of random Hermitian matrices are determined.

34T7079 EXTENDED HÜCKEL MOLECULAR ORBITAL CALCULATIONS

An IBM 7040 program has been adapted for running on the CDC 3600 computer. Molecular orbital calculations are made for fluorides of the oxygen and nitrogen subgroups.

Listed below by title are those programs still in progress at the end of the report year:

B104	COMPUTER SERVICES REPORT FOR LABORATORY ACCOUNTING
B141	DESIGN OF 750-KEV ACCELERATING COLUMN
B142	MONTE CARLO SOLUTION OF A STOCHASTIC DIFFERENTIAL EQUATION
B156	DETERMINATION OF RADIOISOTOPES BY LEAST-SQUARES RESOLUTION OF GAMMA SPECTRA
B158	AN ASYMPTOTIC REGRESSION
B162	CRYSTALLOGRAPHIC D-SPACE PROGRAM
B181	GENERAL LEAST-SQUARES PROGRAM
B186	A THERMAL-ELLIPSOID STEREOGRAPHIC SLIDE PROGRAM
B193	ELECTRODE POTENTIAL VS. POLARIZING CURRENT
B195	SIMULATION OF LABELED MITOSIS CURVES
B196	BAND STRUCTURE CALCULATION
B199	BIG BUBBLE CHAMBER CONVECTIVE FLOW
B203	CRYSTALLOGRAPHIC CONTOUR MAPS
B204	A FIT OF CRYSTAL FIELD EQUATIONS TO MAGNETIC SUSCEPTIBILITY DATA
B205	VAPOR PRESSURE CALCULATIONS
B206	STUDY OF AUTOCORRELATION OF A STATIONARY BIRTH AND DEATH PROCESS
B210	LEAST-SQUARE REFINEMENT PROGRAM
B211	DETERMINATION OF CRYSTAL STRUCTURE
B212	LINEAR ENERGY TRANSFER ANALYSIS
B213	CRYSTALLOGRAPHIC PROGRAMS FOR THE 1130
B216	IRREVERSIBLE TRANSFER IN A BIMETALLIC CELL
B221	CALCULATION OF EXPERIMENTAL CAPTURE CROSS SECTIONS
B222	DETERMINATION OF ISOTOPIC RATIOS WITH MULTICHANNEL ANALYSES
B226	METAL-WATER REACTIONS DURING ACCIDENT
B227	ALGEBRAIC COMPUTATIONS IN COGENT

B230	SINGLE-CRYSTAL NEUTRON DIFFRACTION DATA PROCESSING
B232	PARTICLE MOVEMENT IN A SWARM OF RISING BUBBLES
B235	CORROSION APPROXIMATION
B236	FIT OF RESISTIVITY VS. RADIATION DOSE
B244	ANALYSIS OF STRESS AND STRAIN DATA
B247	A FIT TO REDUCE CROSS SECTIONS
B250	WIENER INTEGRALS AND TAXONOMY
B259	TEMPERATURE DECAY IN A CALORIMETER
B260	NEUTRON DIFFRACTION DATA REDUCTION AND EXTINCTION CORRECTION
B261	OVERLAY SYSTEM FOR B145, MET153, AND B114 PROGRAMS
B262	PROMISE - REACTOR CORE DESIGN
C144	WIDTH CALCULATIONS IN METALS
C146	DIFFUSION KINETICS IV
C147	EXPERIMENTAL DATA ANALYSIS-RESISTIVITY VS. TEMPERATURE
C152	DECAY OF TWO INTERACTING SPECIES
C155	PROTON MAGNETIC RESONANCE LINESHAPE
C157	INTERTHERMOMETER COMPARISON
C161	RESOLUTION CORRECTION
C164	DETERMINATION OF RATE CONSTANTS FOR CHEMICAL REACTIONS
C170	FISSION FRAGMENT CORRELATIONS
C171	FREQUENCY FUNCTIONS OF A LIQUID
C172	ASI MULTIPARAMETER ANALYSIS
C179	SPIN LATTICE RELAXATION IN MÖSSBAUER SPECTRA
C181	COMPUTATION OF SLATER-PARAMETER COEFFICIENTS, ENERGY LEVELS, AND ATOMIC SPECTRA
C186	PARTICLE COUNTS AT SURFACE OF FLUIDIZED BED
C187	CHECKING EQUATIONS FOR ODD U^K MATRIX ELEMENTS
C188	FITTING NEUTRON DIFFRACTION PATTERN

C190	I/O SUBROUTINES FOR SYSTEM 360
C192	CURVE FITTING FUNCTION SPECIFICATION
C194	MEASUREMENTS OF FAST REACTIONS IN RADIATION CHEMISTRY
C196	CALCULATION OF IODINE INHALATION RADIATION DOSES--AD HOC PANEL ON AARR SAFETY EVALUATION
C198	CALCULATION OF RADIATION DOSE RATIOS--AD HOC PANEL ON AARR SAFETY EVALUATION
C200	CONFIGURATION INTERACTIONS WITH f^n CORE
H122	MAP - SPATIAL RECONSTRUCTION OF WIDE GAP SPARK CHAMBER TRACKS
H123	PRINTAP 2
H124	INTERMEDIATE BOSON CROSS-SECTION CALCULATION
H126	GENRAT - SIMULATION OF BUBBLE CHAMBER EVENTS
H127	MAESTRO - A PROGRAM FOR THE REAL TIME GENERATION OF MUSICAL SOUNDS
H128	AUTOMATIC PROCESSING OF LAMBDA-BETA DECAY EXPERIMENT
H129	AUTOMATIC PROCESSING OF SIGMA MAGNETIC MOMENT EXPERIMENT
H130	GRAPHICAL MAN-MACHINE INTERFACING
H131	FILM SCANNER CALIBRATION
I100	DATA ACQUISITION AND/OR TIME-SHARING VIA REMOTE CONSOLE
I101	MONTE CARLO MODEL FOR 3600 OPERATIONS
I102	PERT STUDY FOR SYSTEM/360 ACQUISITION
I104	TOPOLOGICAL PROPERTIES OF TWO-DIMENSIONAL SELF-RESTRICTING MAZES
I106	SELECTIVE DISSEMINATION OF INFORMATION UTILITY ROUTINE
I110	FINGERPRINT CLASSIFICATION AND IDENTIFICATION
I113	SDI MATCHING PROGRAM
I116	TPD BUDGET AND TYPE COUNTING ROUTINE
I117	ORIENTATION AND ANGLE SETTING GENERATION
I118	COMPLEX SPECTRA ANALYSIS IN HUMANS
I119	LOW ENERGY ELECTRON RESPONSE SPECTRA IN SILICON
I120	PATTERN RECOGNITION TEST

P140	CALCULATIONS OF SPIN-SPIN RELAXATION IN FE(NH_4) (SO_4)
P144	MÖSSBAUER OPTIMIZATION
P147	CHOPPER TRANSMISSION ANALYSIS
P153	ABACUS
P154	FOUR-PARAMETER ANALYZER ANALYSIS
P156	PHYLIS LIBRARY TAPE SYSTEM
P160	ASSEMBLER FOR THE IBM 1130
P167	FIT HAMILTONIAN TO SPECTRA
P180	ND 160 COMMUNICATION PROGRAMS VIA B05
R147	COUNTER-CURRENT FLOW DOUBLE PIPE HEAT EXCHANGER PROBLEM
R149	TRAFICORPORATION
R150	SYSTEMS EVALUATION
R151	UO_2 PHONON DISTRIBUTION
R152	CANDID
R154	ROCKET CYCLE ANALYSIS
R155	PRELIMINARY DESIGN OF AN INDUCTION MHD GENERATOR
R157	DOPPLER BROADENED CROSS SECTIONS
R160	LIQUID FILM GENERATOR OPEN AND CLOSED CIRCUIT ANALYSIS
R161	DEFLECTION AND STRESS ANALYSIS FOR THIN PLATES AND TUBES
R163	CANDID1D
R164	MHD CYCLE EFFICIENCY ANALYSIS
R165	MISCELLANEOUS PROGRAMS (AMD PROGRAM LIBRARY)
R166	TRANSCENDENTAL BESSEL EQUATION ROOTS
R167	TRANSPORT DELAY SUBROUTINE
R168	COOLANT EXPULSION STUDIES - DATA REDUCTION
R169	SATURATED - COUNT RATE CALCULATION FOR ACTIVATED LIQUIDS
R171	MISCELLANEOUS REACTOR CALCULATIONS
R172	NUCLEAR SAFETY - ACCIDENT ANALYSIS

R173	MATHEMATICAL RESEARCH AND PROGRAM DEVELOPMENT (REACTOR DESIGN)
R174	PRELER III - PRESSURE AND LEAKAGE RATE TEST FOR EBWR
R175	TECHNICAL PROGRAM COMMITTEE SERVICE
001E6001	ELECTRON MICROPROBE DATA ANALYSIS
003E6009	CONSULTATION ON VARIOUS CRYSTALLOGRAPHIC PROGRAMS
004E6010	CONSULTATION ON VARIOUS CRYSTALLOGRAPHIC PROGRAMS
06E7016	COMPUTER SERVICES REPORT FOR LABORATORY ACCOUNTING
08E7037	LEAST-SQUARES CALCULATION OF VAPOR PRESSURE
09E7030	PLOT OF ACTUAL AND PROJECTED PROGRAM COSTS
11E7041	HIGH-TEMPERATURE THERMODYNAMIC FUNCTIONS
13E7042	RESISTIVITY OF THIN FILMS
15E7051	METAL-WATER REACTIONS DURING ACCIDENT
17E7056	FOURIER ANALYSIS OF CRYSTAL LATTICES IN TWO AND THREE DIMENSIONS
18E7060	ANALYSIS OF EBR2 FUEL PIN SWELLING
19E7062	CRYSTALLOGRAPHIC D-SPACE PROGRAM
20E7063	HEATING RATES IN A^2R^2 SUPPORT STRUCTURES
21E7064	CALCULATION OF STORED ENERGY IN RADIATED MATERIALS
22E7067	APPLIED PROGRAMMMING EFFORT
23E7074	HFIR IBT-SPOT CODE
24E7075	PLUME RISE
25E7080	STATISTICAL ANALYSIS OF PARTIALLY ORDERED DEFECTS IN NONSTOICHIOMETRIC IONIC CRYSTALS
26E7085	CALCULATION OF DAMAGE RATE DERIVATIVES
27E7090	DIRECT METHOD USING TANGENT FORMULA
28E7091	ANALYSIS OF STRESS-STRAIN DATA
01R6005	TRANSPORT THEORY SEMINARS
02R7001	RE138 and RE171 FOR THE 3600
04R7010	PETER

05R7011	NEUTRONICS PREPARATION INPUT
06R7012	NEUTRONICS PREPARATION
08R7029	STOCHASTIC PROBLEMS IN TRANSPORT THEORY
09R7047	AARR PRESSURE VESSEL CONTAINMENT POTENTIAL
11R7068	GROWTH OF TWO COMPETING POPULATIONS
01S6001	PROGRAMMING AND COMPUTING FOR THE FAST NEUTRON HODOSCOPE
03S7002	ANALYSIS OF BINARY NUCLEAR FISSION DATA TAPES
04S7007	LIBRARY DEVELOPMENT FOR S/360
08S7013	LINKAGE FROM PL/I TO FORTRAN AND VICE VERSA
14S7061	INTRINSIC MULTIPROCESSOR SIMULATION
15S7066	ANGULAR DISTRIBUTION FOR FISSION FRAGMENTS
16S7076	FSCOPE - OSCILLOSCOPE AND LIGHT PEN DISPLAY
17S7081	BINARY ("PSEUDO-BCD") TAPE ANALYSIS PROGRAM
18S7082	BINARY DATA TAPE ANALYSIS
19S7083	LIBRARY SERVICES SUBROUTINE PACKAGE
20S7084	JOURNAL RENEWAL SYSTEM
04T7008	ARGONNE CODE CENTER
05T6003	COMBINED CONDUCTION-RADIATION PROBLEM, INCLUDING TRANSIENTS
06T7010	TRAJECTORY CALCULATIONS FOR A MAGNETIC SPECTROMETER
08T7019	CHEMICAL EQUATION TRANSLATOR
09T7022	BUBBLE CHAMBER FLOW DYNAMICS
11T7024	CALCULATION OF CUBIC HARMONICS
13T7026	CONFIGURATION INTERACTIONS - FANO
16T7032	CALCULATION OF ELECTRONIC TRANSITION PROBABILITIES
17T7033	CONVERSION AND REDUCTION OF RIDL CHANNEL ANALYZER DATA
18T7036	DETERMINATION OF FERMI SURFACE FROM DE HAAS VAN ALPHEN MEASUREMENTS
19T7038	THERMOCOUPLE CALIBRATION PROGRAM
20T7049	POLYNOMIAL FACTORIZATION

21T7050	PROGRAMMING CONSULTANT SERVICES
22T7052	DIFFERENTIAL EQUATION SOLVER
23T7054	TABULATION OF TWO FUNCTIONS OCCURRING IN MESIC X-RAY CALCULATIONS
24T7058	FISSION FRAGMENT MATRIX ANALYSIS
25T7059	THERMO-ELECTRIC POWER CALCULATIONS
26T7065	USE OF PROGRAM GERT
27T7068	MODEL OF BIOLOGICAL SYSTEM
29T7070	ESR LINE SHAPES IN MH_2AO_4 COMPOUNDS
32T7077	REDUCTION OF GROUP REPRESENTATIONS
33T7078	STRESS, STRAIN, AND CREEP COMPUTATIONS
35T7086	MONTE CARLO CALCULATIONS
36T7087	FOURIER TRANSFORMS OF TIME-LIMITED SIGNALS
37T7088	PROGRAM DEVELOPMENT AND DEBUGGING
39T7092	AN ALTERNATE PROCEDURE FOR CALCULATING ESR LINE SHAPES

DIGITAL COMPUTER OPERATIONS

In 1966-1967 the CONTROL DATA 3600 and IBM System 360/50 computers performed the bulk of the computational assistance to Argonne's scientists and technicians.

IBM System 360

The Model 50 installed in July, 1966 functioned as a single computer until June 12, 1967, at which time it was shut down to be joined by the Model 75 and a second card reader punch, two additional printers, disks, data cells, drum, and other equipment. It furnished a transition to the later System 360 configuration and a training period as well as a period of useful computations, and was operated approximately one and one-half shifts per day.

The number of useful computations averaged several hundred per week during the transition period.

CDC 3600

The CDC 3600 was operated continuously. Turnaround for the shorter computations during the normal day hours, Monday through Friday, varied with the length of the queue and other factors from one and one-half hours to three hours.

During the daytime and the early evening, computations of less than five minutes' total duration were expedited; when no jobs of this category were available, jobs of less than ten minutes' total duration were run. Longer jobs and attended runs were completed as time permitted. During a normal Monday through Friday, 200 to 250 jobs were run between 8:30 AM and 5:00 PM; some on-line systems development work was also scheduled during these hours. A feature of the Monday-Friday evening operations was the provision for several expedited turnarounds in the 6:00 PM to 10:00 PM hours. Programmers on a "crash" schedule were thus able to accomplish their work faster. An average of 150 jobs of varying lengths were completed during the remaining evening and early morning hours. A similar arrangement was provided on week-ends between 2:00 and 5:00 PM. Total useful production for the year was 7154 hours, or 82% of the available time in the year. Unused time totaled 391 hours, nearly all of which was in the Thanksgiving, Christmas, and New Year holiday shutdowns plus the shutdowns resulting from the January, 1967 blizzard, and building air-conditioning modification in March, 1967.

IBM 1401

The IBM 1401 handled most of the miscellaneous tape-to-card, tape-to-tape, and tape-to-printer requests daily from the Argonne (reactor) Code Center and other individual sources.

CDC 160-A

Two CDC 160-A computers primarily perform input and output functions for the CDC 3600. One utilizes the 828 disk for input to and output from the

3600; the input data immediately becomes available to the 3600 for computation and the output to the 160-A for printing. Three printers are shared by both 160-A's, while another is connected only to the off-line 160-A; two card readers are connected to the off-line 160-A, and one of the two is also connected to the Satellite 160-A. Punched output is performed by the off-line 160-A or by the IBM 1401.

Remote Station 160-A's

A microwave connection to a 160-A computer in the High Energy Physics area is tied into the Satellite 160-A; transmission of data is accomplished several times daily during the prime shift to and from the 3600 by means of a tape-to-tape copying routine. Because of volume, longer 3600 jobs are transmitted to the computer center by courier each afternoon at the end of the prime shift and returned complete with printout by truck the next morning.

The 160-A computer in the High Energy Physics Building is engaged in various relatively routine data editing and data transfer problems, in addition to its transmission assignments. Some customer programming of small jobs is done also.

The 160-A computer in the Reactor Divisions Building is extremely busy with smaller programs, mostly written by and for Reactor personnel who wish to perform their own computations. There are also important duties involving active experiments in the area. Recently this computer has averaged over 100 hours per week of useful computations, including much hard copy plotting with an on-line Calcomp incremental plotter.

Maintenance

Maintenance of the various computers is accomplished by five Control Data Corporation engineers permanently at Argonne, and six IBM engineers full and part time. Single shift maintenance during the prime shift, Monday through Saturday, was purchased from IBM for the System 360. Single shift maintenance for the prime shift, Monday through Friday, was purchased for the 1401 and other IBM equipment. Single shift maintenance Monday through Friday for the CONTROL DATA 3600 and two 160-A computers in the Applied Mathematics Building computer complex and the two remote 160-A computers was purchased. The CDC computer arrangements were revised following detailed studies of the relative costs and advantages of the various plans available, resulting in a significant cost reduction in maintenance charges for CDC equipment.

Maintenance of plotters and other peripheral equipment is performed by Argonne personnel who have been trained in the work.

Graphic Output

Graphic output equipment includes the CDC Cathode Ray Tube DD80 on-line from the CDC 3600 to 35mm film, and two off-line Calcomp digital plotters, plus an on-line Calcomp plotter connected to the Reactor 160-A. All devices experienced heavy usage. The single off-line Calcomp plotter was completely saturated with a queue that occasionally exceeded 48 hours and with an average usage of 140 hours per week. Consequently another was added during the year.

Cathode Ray Tube (CRT) output is being encouraged by the faster development of film through use of an Eastman Kodak Recordak, which has been modified to accept the take-up reel of the CRT film camera and which can develop 5 feet of film per minute. Volume averages 100 feet of film per day, representing output of approximately 1500 pictures — from 5% to 10% of the jobs run on the 3600.

General

The hardware of the CDC and IBM computers has been very reliable, resulting, for example, in a CDC 3600 record of availability of over 90%.

Tape reel testing and retesting continues to be necessary, and many man hours a week are required for that operation.

OPERATIONS EXPERIENCE DURING THE PERIOD JULY 1, 1966 - JUNE 30, 1967

	Hours						
	Charged & Sustaining	Setup	Uncharged	Maintenance Sched.	Maintenance Unsched.	Unused	Engineering
CDC 3600	6463.9	187.2	199.2	631.4	152.1	391.2	43.3
IBM System 360/50	1186.1	17.5	40.5	144.8	69.4	1849.5	517.9
CDC 160-A Off-line	8328.6	0	0	110.9	18.2	239.6	0
CDC 160-A High Energy Physics	2732.8	0	0	140.0	19.7	4043.4	4.8
CDC 160-A Reactor	3093.2	0	0	177.33	148.57	3541.2	4.8
IBM 1401	4431.0	0	36.0	48.0	54.0	4221.0	0

1a. Charged - All computing and processing of data including the development of computer programs, except as noted below. A transfer of funds is involved for all time in this category. (Research time used by the Applied Mathematics Division staff is included here.)

1b. Sustaining - Use of authorized AMD personnel for the following purposes: developing and testing of programming systems supporting the use of the computer, demonstrations, training, and reliability testing of hardware and software, except as noted below.

2. Setup - Time consumed in setting up tapes and equipment for a "batch" of jobs processed by the monitor system.

3. Uncharged - Computer use for reruns attributable to the malfunction of the computer, peripheral equipment, supplied or AMD-supported programming systems, or to AMD clerical or operating errors.

4. Scheduled Maintenance - Time consumed for scheduled preventive maintenance by customer engineers.

5. Unscheduled Maintenance - Time elapsed between the request for, and the completion of, corrective action required by equipment malfunction.

6. Unused - Computer time not otherwise accounted for.

7. Engineering - Time consumed for Engineering changes, new attachments, and acceptance testing, by either ANL or computer manufacturer's personnel.

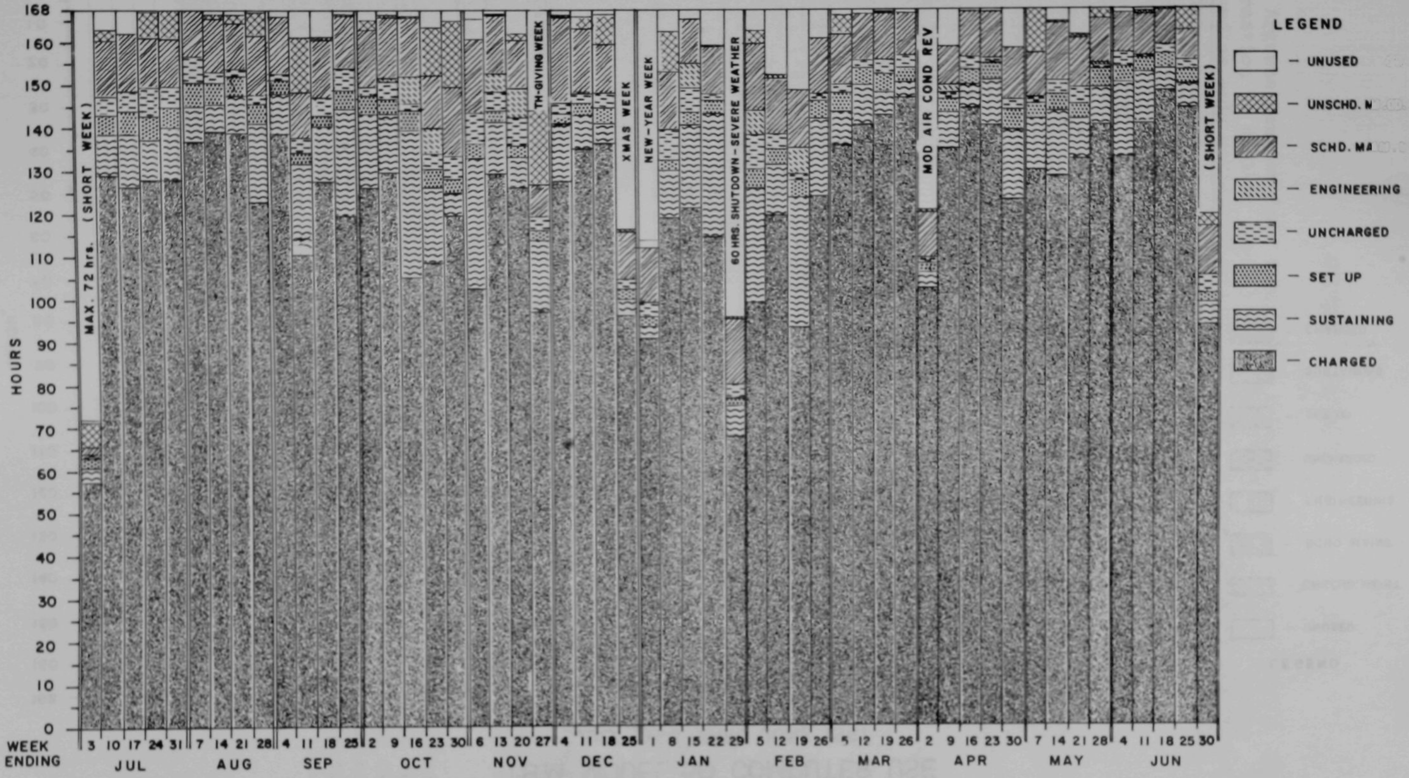
Other equipment, for which formal statistics are not maintained:

Calcomp Plotters - Operated 16 to 20 hours per day, 7 days per week.

CDC 160-A (Satellited to 3600) - Used approximately same hours as the 3600.

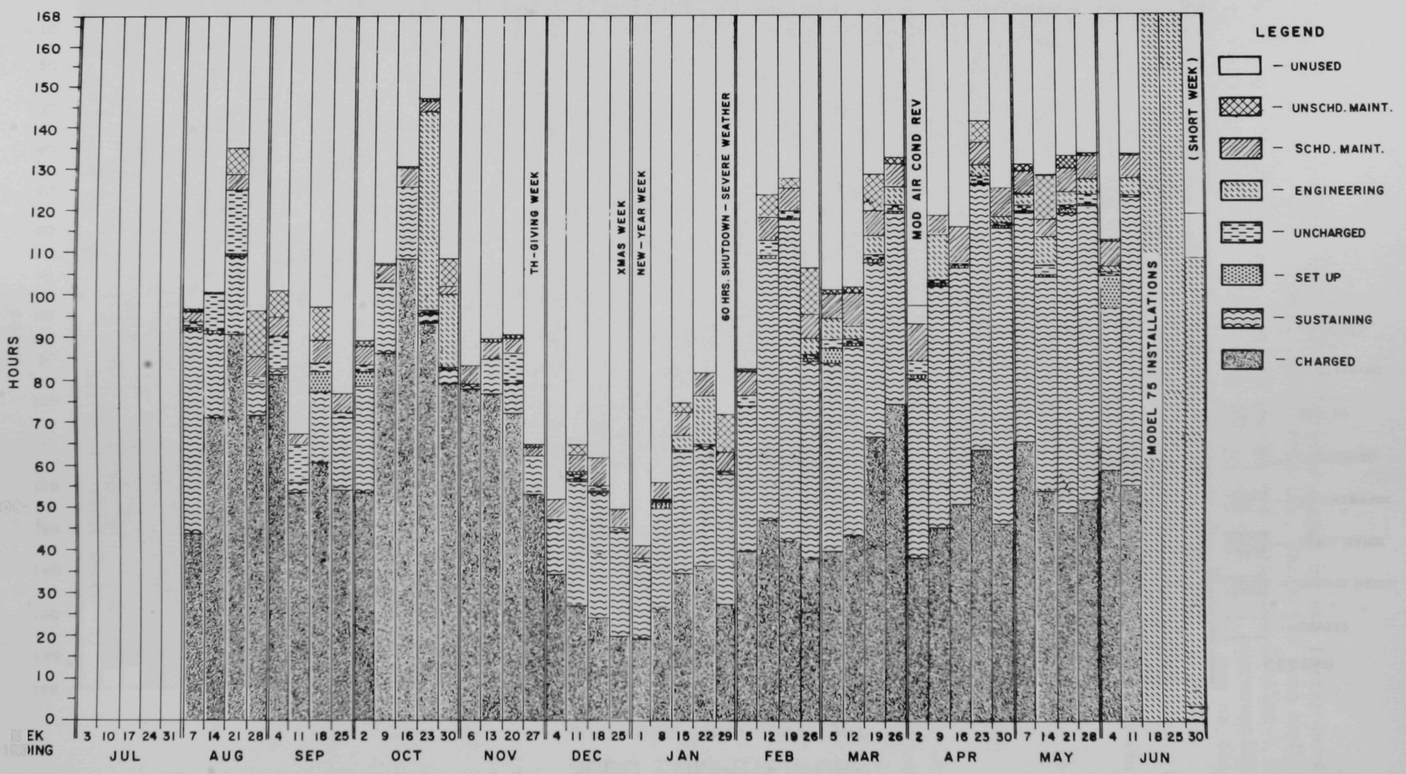
3600 COMPUTER USE

JULY 1966 THRU JUNE 1967



IBM MODEL 50 COMPUTER USE

JULY 1966 THRU JUNE 1967



ARGONNE CODE CENTER

The Argonne Reactor Code Center, established in 1960, is a central agency for information on nuclear physics and reactor design computer programs. The Center handles only unclassified computer programs and restricts the distribution of Naval Reactor code packages to United States citizens for domestic applications. The scope of this activity includes:

1. the collection of reactor design computer programs and their assimilation in the Center's library;

2. the reproduction and distribution of code package material for the programs in the Center's library;

3. the preparation, editing, and publication of a program abstract describing each program contained in the Center's library;

4. the maintenance and North American distribution of ENEA Computer Programme Library programs and code package material (ENEA is the European Nuclear Energy Agency);

5. The initiation and encouragement of and assistance in the development of standards and practices, particularly in the areas of program documentation and programming practices, that will facilitate the exchange of computer programs.

The program abstracts published under category (3) are distributed, upon request, to members of the Mathematics and Computation and the Reactor Physics Divisions of the American Nuclear Society by the Society, and to others by the Center. Argonne Reactor Code Center code package material is deposited with the ENEA Computer Programme Library for European distribution.

During the year the Center has published and distributed program abstracts for 51 program additions to the library, 33 ENEA program abstracts, and two revisions. 741 program packages have been dispatched over this same period, including 612 to requestors within the United States. Universities received 135 program packages.

Cooperative work continued with the ANS-10 Standards and Benchmark Problem Committees of the American Nuclear Society's Mathematics and Computation Division. This work involves the preparation of a set of programming guidelines to facilitate program-computer interchange, a listing of FORTRAN compiler implementation idosyncracies to be considered in effecting the interchange, and a collection of benchmark problems in the area of reactor physics.

PUBLICATIONS AND PAPERS

Publications

1) A. DeVolpi(1), K. G. Porges(1), G. C. Jensen, COINC, Computer Code for Reduction of Coincidence Counting, Nucl. Sci. Eng., 25, 306 (July 1966) (Note).

2) Forrest Salter, Integrated Circuits Quickly Assembled, Electronics, 39, 103-104 (July 1966) (Note).

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31) The Argonne Reactor Computation System ARC, by C. N. Kelber(5), G. C. Jensen, L. C. Just, and B. J. Toppel(5). Conference on Research Reactor Utilization and Reactor Mathematics, Mexico City, May 1967.

32) Generation of Multigroup Cross Sections Using a Coupled MC^2-THERMØS Code, by D. A. Sargis(5), B. J. Toppel(5), and A. L. Rago. Conference on Research Reactor Utilization and Reactor Mathematics, Mexico City, May 1967.

33) Use of the ELMOE-SNARG Programs to Study Details of Neutron Spectra through Regions of Resonance Scattering Media, by D. Meneghetti(5), A. L. Rago, and K. E. Phillips(5). Conference on Research Reactor Utilization and Reactor Mathematics, Mexico City, May 1967.

34) Automatic Analysis of Bone Autoradiographs, by J. W. Butler, Elizabeth Lloyd(9), and J. H. Marshall(9). Symposium on Automatic Photointerpretation, Washington, D.C., May 31-June 2, 1967.

35) POLLY, An Interactive System for Bubble Chamber Film Measurement, by R. K. Clark, D. Hodges, J. G. Loken(2), B. Musgrave(2), P. Pennock, B. Phillips(2), R. J. Royston(2), R. H. Wehman, and G. W. Wittmus. Symposium on Automatic Photointerpretation, Washington, D.C., May 31-June 2, 1967.

36) Automatic Processing of 1000 Marmoset Spreads, by J. W. Butler, M. K. Butler, and Barbara Marczynska(10). Conference on Data Extraction and Processing of Optical Images in the Medical and Biological Sciences, New York Academy of Sciences, New York, June 5-7, 1967.

37) Foundations of the Theory of Branching Processes, by Joseph M. Cook. SIAM 1967 National Meeting, Washington, D.C., June 12, 1967.

38) Status Report: Argonne Code Center, by Margaret K. Butler. ANS 1967 Annual Meeting, San Diego, California, June 14, 1967.

39) Convergence Rates for Empirical Bayes Two-Action Problems, by J. Van Ryzin and M. V. Johns, Jr.(6). 115th Meeting of the Institute of Mathematical Statistics, University of Montana, Missoula, Montana, June 15-17, 1967.

(1) Biological and Medical Research Division
(2) High Energy Physics Division
(3) Physics Division
(4) Combustion Engineering Inc., Windsor, Connecticut
(5) Reactor Physics Division
(6) Stanford University
(7) Reactor Engineering Division
(8) Bell Telephone Laboratories
(9) Radiological Physics Division
(10) Presbyterian-St. Lukes Hospital

SEMINARS AND SYMPOSIA

Applied Mathematics Division Seminars

July 7, 1966	Approximate Computational Solution of Nonlinear Parabolic Partial Differential Equations by Linear Programming, by Prof. J. Ben Rosen, Chairman, Computer Science Department, University of Wisconsin, Madison, Wisconsin.
July 14, 1966	On the Newton-Raphson Method for Nonlinear Equations, by Prof. Adi Ben-Israel, Department of Systems Engineering, University of Illinois Circle Campus, Chicago, Illinois.
July 21, 1966	An Iterative, Quadratically Convergent Numerical Method for Solving the Hartree-Fock-Roothaan Equations: An Extremum Problem with Constraints, by Dr. W. Roy Wessel, Research Associate, Department of Physics, University of Chicago, Chicago, Illinois.
July 28, 1966	Analytic Continuation of the Resolvent Kernel and Exponential Decay of Solutions of the Wave Equation, by Prof. Dale Thoe, Department of Mathematics, Purdue University, Lafayette, Indiana.
August 11, 1966	Stochastic Models in Biology, by Prof. Joseph Gani, Chairman - Department of Mathematical Statistics, University of Sheffield, Sheffield, England and Visiting Professor at Michigan State University, Department of Statistics and Probability, East Lansing, Michigan.
August 19, 1966	The IIT Time Sharing System, by Mr. W. S. Worley, Assistant Director for Systems, Information Processing Center, Illinois Institute of Technology, Chicago, Illinois.
August 25, 1966	The Numerical Integration of Stiff Ordinary Differential Equations, by Prof. C. W. Gear, Department of Computer Science, University of Illinois, Urbana, Illinois, and Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
September 15, 1966	Topological Network Theory, by Prof. Paul Slepian, Rensselaer Polytechnical Institute, Troy, New York and Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
September 22, 1966	Automatic Data Retrievers, by Dr. Franz L. Alt, Mgr. Inf. Systems - Office of Std. Ref. Data, National Bureau of Standards, Washington, D.C.

October 6, 1966	Convergence of a Quadrature Formula in the Presence of a Singularity, by Prof. Walter Gautschi, Computer Sciences Department, Purdue University, Lafayette, Indiana.
October 13, 1966	The Problems of Software Design, Construction, and Implementation of Multiple Terminal Time Sharing Systems in a Scientific Environment, by Mr. John H. Morrissey, Morrissey Associates, Inc., New York City.
October 20, 1966	Optical Scanning Devices, by Dr. H. P. Mansberg, Cutler-Hammer Airborne Instruments Laboratory, Dept. of Medical and Biological Physics, Long Island, New York.
October 27, 1966	On a Canonical Representation of Scattering Matrices, by Prof. Alberto Gonzalez-Dominquez, Visiting Professor, Department of Mathematics, University of Chicago, Chicago, Illinois.
November 10, 1966	Steady-State Wave Propagation in Homogeneous Anisotropic Media, by Prof. Calvin Wilcox, Mathematics Department, University of Arizona, Tucson, Arizona.
November 17, 1966	Branching Random Walks and Cascade Processes, by Prof. Peter Ney, Department of Mathematics, University of Wisconsin, Madison, Wisconsin.
December 1, 1966	Some Questions of Lie Algebras, by Dr. N. Burgoyne, Mathematics Department, University of Illinois Circle Campus, Chicago, Illinois.
December 8, 1966	Nonlinear Wave Propagation, by Prof. Ellis Cumberbatch, Division of Mathematical Sciences, Purdue University, Lafayette, Indiana.
December 9, 1966	Concepts of Intrinsic Multiprocessing, by Mr. Richard A. Aschenbrenner, Applied Mathematics Division, Argonne National Laboratory; Dr. Michael Flynn, Northwestern University and Dr. George A. Robinson, University of Wisconsin - both consultants with Applied Mathematics Division, Argonne National Laboratory.
December 15, 1966	Block Generalizations of Some Gerschgorin-Type Theorems, by Dr. R. L. Johnston, Department of Mathematics, University of Toronto, Toronto, Ontario, Canada.
December 22, 1966	Matrices with Dominant Principal Diagonal and Some Applications, by Prof. G. Baley Price, Chairman, Department of Mathematics, University of Kansas, Lawrence, Kansas.

January 10, 1967	*<u>The Mathematical Status of the Pseudo-Steady State Hypothesis in Chemical Kinetics</u>, by Dr. Rutherford Aris, Professor Chemical Engineering, Institute of Technology, University of Minnesota, Minneapolis, Minnesota.
January 19, 1967	<u>The General Root Powering Method for Finding the Zeros of Polynomials on Present and Future Generation Computers</u>, by Dr. E. H. Bareiss, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
February 23, 1967	<u>Least Squares Monte Carlo Methods for Linear Problems</u>, by Dr. John H. Halton, Mathematics Research Center (U.S. Army), University of Wisconsin, Madison, Wisconsin.
March 2, 1967	<u>Algebras of Germs of Fourier Transforms</u>, by Prof. Meyer Jerison, Department of Mathematics, Purdue University, Lafayette, Indiana.
March 9, 1967	<u>Recent Advances in Image Processing</u>, by Mr. James Butler, Applied Mathematics Division, Argonne National Laboratory.
March 14, 1967	<u>Optically Accessed Memories and Interference Photography</u>, by Mr. Jerry L. Reynolds, IBM Product Development Laboratory, Poughkeepsie, New York.
March 16, 1967	<u>Perceptron Progress</u>, by Mr. Kurt Enslein, Consultant, Rochester, New York.
March 23, 1967	<u>Electromagnetic Levitation Forces</u>, by Dr. W. E. Smith, Applied Mathematics Division, Argonne National Laboratory.
March 29, 1967	<u>PEPR - Precision Encoding and Pattern Recognition</u>, by Dr. Irwin Pless, Particle Accelerator Division, Argonne National Laboratory.
April 27, 1967	<u>Pattern Recognition by Digital Computer; Artificial Intelligence?</u>, by Dr. Lawrence Stark, University of Illinois Circle Campus, Chicago, Illinois.
May 1, 1967	<u>What Next in PL/I?</u>, by Dr. M. Douglas McIlroy, Bell Telephone Laboratories, Murray Hill, New Jersey.
May 5, 1967	<u>Eliminating Monotonous Mathematics with FORMAC</u>, by Mr. R. G. Tobey, International Business Machines Corporation, Cambridge, Massachusetts.

*This was a joint seminar with the Biological and Medical Research Division, held in Building 202.

May 18, 1967	Approximate Solutions of Integral and Operator Equations, by Prof. P. M. Anselone, Mathematics Research Center, The University of Wisconsin, Madison, Wisconsin and Mathematics Department, Oregon State University, Corvallis, Oregon.
May 25, 1967	*Models of Intelligence, by Prof. Leonard Uhr, Computer Science Department, University of Wisconsin, Madison, Wisconsin.
June 1, 1967	Coding of Mathematical Functions and Error Analysis, by Mr. Hirondo Kuki, Institute for Computer Research, University of Chicago, Chicago, Illinois.
June 8, 1967	Symbolic Control - The Application of Computers to Numerical Control, by Mr. Benjamin Mittman, Director of Vogelback Computing Center, Northwestern University, Evanston, Illinois.
June 15, 1967	On Analytic Perturbation Theory, by Prof. Peter Lancaster, Department of Mathematics, University of Calgary, Calgary, Alberta, Canada.
June 22, 1967	Time Dependent Transport Problems, by Dr. Hans G. Kaper, University of Groningen, Groningen, The Netherlands, and Visiting Associate Professor, Stanford University, Mechanical Engineering Department, Nuclear Division, Stanford, California.
June 27, 1967	Almost Diagonal Matrices with Multiple or Pathologically Close Eigenvalues, by Prof. J. H. Wilkinson, National Physical Laboratory, Mathematics Division, Teddington, Middlesex, England.
June 28, 1967	Limiting Accuracy Attainable in Computed Inverses, by Prof. J. H. Wilkinson, National Physical Laboratory, Mathematics Division, Teddington, Middlesex, England.
June 29, 1967	Remarks on Compiler Construction, with Particular Attention to Symbolic Addresses, by Prof. Robert Floyd, Department of Computer Science, Carnegie Institute of Technology, Pittsburgh, Pennsylvania.

*This was a joint seminar with the Physics Division, held in Building 203.

Applied Mathematics Division Special Interest Seminars

July 21, 1966	Design Considerations in the SIGMA 7 and Announcement of New Small Scale Computer, by Mr. Sol Vasloff, Advanced Products Manager, Scientific Data Systems, Santa Monica, California.
October 7, 1966	PL/I. What is it? Why use it? Where is it now? by Dr. M. Donald MacLaren, Applied Mathematics Division, Argonne National Laboratory, Argonne, Illinois.
January 3, 1967	Tasker Instrument Series 9,000 Modular Display System, by Mr. M. E. Forgey, Information Systems, Tasker Instruments Corporation, Van Nuys, California.
January 6, 1967	Capabilities of the S-C 4060 Stored Program Recording System, by Mr. W. B. Grawe, District Manager Stromberg-Carlson Data Products Division, Hinsdale, Illinois.
January 11, 1967	Computer Controlled Displays from Information Displays, by Mr. C. Machover, Information Displays, Inc., Mt. Vernon, New York.
February 15, 1967	The BR-90 Visual Analysis Console, by Mr. Frank Beach, Bunker-Ramo Defense Systems Division, Canoga Park, California.
February 20, 1967	Adaptive Microprogrammed Control System, by Mr. Frank Williams, Engineering Manager Federal Systems Division, IBM.
March 24, 1967	Use of the IBM 2280 Film Recorder at Chemical Abstracts Service, by Mr. Frank Anzelmo, Systems Development Department, Chemical Abstracts Service, Columbus, Ohio.
June 7, 1967	DEC Graphic Hardware, by Mr. Barry Wesler, Digital Equipment Corporation, Maynard, Massachusetts.
June 23, 1967	A special showing of a short film shown at the San Diego American Nuclear Society Meeting depicting joint IBM-AI cross section work utilizing the 2250 Graphic Display.

Transport Theory and Stochastic Processes

A weekly seminar lecture series started on March 23, 1966 is continuing, with Dr. J. E. Moyal in charge. Seminars given by Dr. Peter J. Brockwell of the Applied Mathematics Division, Argonne National Laboratory; Prof. T. W. Mullikin of Purdue University; Dr. Erwin H. Bareiss, Applied Mathematics Division, Argonne National Laboratory; Prof. David M. Topping, University of Washington, Seattle, Washington; Dr. Ibrahim K. Abu-Shumays, Applied Mathematics Division, Argonne National Laboratory; Dr. J. M. Cook, Applied Mathematics Division, Argonne National Laboratory; Mr. Harold Greenspan, Applied Mathematics Division, Argonne National Laboratory; Dr. Hans G. Kaper, Visiting Professor, Stanford University.

Conference on Gerschgorin and Lyapunov Methods in Matrix Theory

A number of leading research workers in the area of Gerschgorin and Lyapunov methods in matrix theory met as invited participants in a conference at Argonne on March 30-31, 1967. Each formal presentation by a speaker on his own contributions in the field was followed by a discussion period.

The matrix computations discussed often arise in physical circumstances from some stability consideration. Control devices must be designed so that perturbations will be damped. The related mathematical requirement is that eigenvalues of an associated matrix be located in the left half of the complex number plane. Lyapunov in 1893 contributed a fundamental technique for determination of a matrix's stability property. Olga Taussky, one of the conference participants, significantly generalized this result in a lecture given at a matrix conference at Gatlinburg in April 1961. Many others at the Argonne conference have published in this area, so one of the aims was that an attempt be made to complete the theory to a computationally effective state.

Another type of location theorem for eigenvalues is due to Gerschgorin. A significant extension of this theory was studied by R. S. Varga, one of the conference organizers, using diagonal similarities to improve estimates. The original results are also important in error analyses of computing methods. Another attendee, H. W. Wielandt, has published extensively on other techniques for eigenvalue location.

Finally, a basic problem in the solution of linear equations is that of equilibration, and this was at least a peripheral subject for consideration at the conference.

Those participating in the conference were: H. A. Antosiewicz (University of Southern California), R. C. F. Bartels (University of Michigan), F. L. Bauer (Stanford University and Technische Hochschule, Munich), H. F. Bohnenblust (California Institute of Technology), A. T. Brauer (University of North Carolina), D. H. Carlson (Oregon State University), W. Givens (Argonne National Laboratory), A. J. Hoffman (International Business Machines Corporation), A. S. Householder (Oak Ridge National Laboratory), R. L. Johnston (University of Toronto), B. W. Levinger (Case Institute of Technology), Helen Medley (Kent State University), N. E. Nirschl (St. Norbert College), H. Schneider (University of

Wisconsin), J. Todd (California Institute of Technology), Olga Taussky Todd (California Institute of Technology), R. S. Varga (Case Institute of Technology), H. W. Wielandt (University of Wisconsin and University of Tubingen), C. H. Wilcox (University of Arizona), J. H. Wilkinson (Stanford University and the National Physical Laboratory).

Mathematical Methods of Quantum Theory

A working seminar series started on March 29, 1966 is continuing, with Dr. J. E. Moyal in charge. Seminars given by Mr. Ernest Thieleker of the Applied Mathematics Division, Argonne National Laboratory; Dr. James C. T. Pool, Applied Mathematics Division, Argonne National Laboratory; Prof. Arlan Ramsay, University of Rochester, Rochester, N.Y.

Knowledge from Ignorance

This is a regular series of discussions on computer-based data acquisition and analysis systems, beginning October 12, 1966 and conducted by Mr. James Butler. Mr. Richard A. Aschenbrenner, Mr. Richard Mueller, Mr. Robert Vonderohe, Mr. Melvin Storm, Mr. David Jacobsohn, Mr. Charles Cohn (RP), Dr. Roy Wessel, all of Argonne National Laboratory.

Conference on Time-Sharing

A two-day conference to discuss time-sharing systems for the IBM 360, model 50 digital computer was held in the Applied Mathematics Division, October 31-November 1, 1966. With these systems, users at perhaps several dozen remote operating consoles are able to solve problems simultaneously. They thus avoid waiting in line for traditional serial processing of data. A number of conversational languages have coincidentally been developed to make communication easier between man and machine.

In each cycle of a time-sharing system, the control program allocates individual time slots to users. The slot is long enough for a fair amount of processing or computation, but the complete cycle is still short enough that there is very little apparent waiting on the part of the human. Such systems are particularly appropriate for solving short problems, but are quite inefficient and slow for longer computations.

Representatives from about 15 organizations with some 9 different time-sharing systems attended the conference. Although a particular machine was the center of discussion, the techniques developed apply to many others as well.

A bound report entitled "Conversation with a 50" is available on request.

Spectral Theory, C*-Algebras, and Quantum Logics

This is a weekly seminar lecture series on the above topic, starting in November, 1966, with Dr. J. E. Moyal in charge.

University and Symposium Presentations

The Business Education Teachers Responsibilities in Teaching Data Processing, by Clifford G. LeVee. Northern Illinois University, DeKalb, Illinois, July 6, 1966.

Compound Sequential Bayes Learning Procedures, by J. VanRyzin. Stanford University, Stanford, California, July 21, 1966.

On Classification Procedures Using Non-parametric Density Estimation, by J. Van Ryzin.
- Brookhaven National Laboratory, July 20, 1966.
- Dept. of Statistics, Stanford University, October 11, 1966.
- Dept. of Statistics, University of Missouri, December 13, 1966.
- Dept. of Statistics, University of Wisconsin, January 18, 1967.
- Dept. of Statistics, University of California, February 14, 1967.

On the Structure of the 3-Dimensional Transport Operator, by E. Bareiss. Josef Stefan Institute, Ljubljana, Yugoslavia, September 5-8, 1966.

Numerical Solution of Polynomial Equations by the General Root Powering Method, by E. Bareiss. Josef Stefan Institute, Ljubljana, Yugoslavia, September 5-8, 1966.

The Generalized Root Powering Method and the Solution of Polynomial Equations on Present and Future Generation Computers, by E. Bareiss.
- Miami University, Oxford, Ohio, October 4, 1966.
- The University of Iowa, Iowa City, Iowa, November 10, 1966.
- The University of Texas, Austin, Texas, December 1-3, 1966.
- Northern Illinois University, DeKalb, Illinois, December 6, 1966.

The Application of Hybrid Computers to Nuclear Reactor Calculations, by L. Bryant. Joint ANS-Pennsylvania State University Graduate Student Seminar, Pennsylvania State University, University Park, Pennsylvania, October 1966.

Careers in Mathematics, by M. Butler. St. Francis Academy, Joliet, Illinois, November 3, 1966.

The Generation of Musical Sounds, by R. Clark. University of Wisconsin, Electrical Engineering Dept., Madison, Wisconsin, November 17, 1966.

Optimization in Decision Processes, by J. Van Ryzin, Dept. of Mathematics, University of Rochester, December 15, 1966.

Digital Integrated Circuits, by Forrest Salter. Carnegie Institute of Technology, Pittsburgh, Pennsylvania, December 15, 1966. Also: ANL Physics Division Colloquium, January 20, 1967.

Statistical Classification Procedures Using Density Estimation, by J. Van Ryzin. Dept. of Mathematics, University of Wisconsin, Milwaukee, Wisconsin, December 16, 1966.

Hybrid Computer Applications, by L. Bryant. University of Illinois, Urbana, Illinois, January 5, 1967.

Design Considerations for Problem-Oriented Digital Systems, by D. Jacobsohn. The University of Iowa, Iowa City, Iowa, January 12, 1967.

Some New Results in Empirical Bayes Finite Action Problems, by J. Van Ryzin. Dept. of Mathematics, Ohio State University, Columbus, Ohio, January 20, 1967.

Applications of Optical Scanning for Business and Science, by Donald Hodges. Symposium on Applications of Optical Scanning for Business and Science, Illinois Institute of Technology, Chicago, Illinois, February 18, 1967.

Machine Classification of Fingerprints, by C. B. Shelman. First National Symposium on Law Enforcement, Science, and Technology, Illinois Institute of Technology Research Institute, Chicago, Illinois, March 7-9, 1967.

Optical Scanning in Medicine and Biology, by J. W. Butler. First National Symposium on Law Enforcement, Science, and Technology, Illinois Institute of Technology Research Institute, Chicago, Illinois, March 7-9, 1967.

A Sequential a posteriori Updating Convergence Algorithm for Pattern Recognition, by J. Van Ryzin, Dept. of Statistics, Stanford University, Stanford, California, March 14, 1967.

The Influence of Machine Design on Numerical Algorithms, by W. J. Cody. Purdue University, Computer Science Department Seminar, Lafayette, Indiana, March 20, 1967.

Is Two Odd or Even? by Robert J. Thomas. Illinois State University Mathematics Seminar, April 25, 1967. Also: Talk to university at large on "non-mathematical computer applications."

The General Root Powering Method for Finding Zeros of Polynomials (and Analytic Functions), by E. Bareiss. The University of Chicago, Chicago, Illinois, May 10, 1967.

Multiplicative Transport Processes in One Dimension, by P. J. Brockwell. Purdue University, Lafayette, Indiana, May 25, 1967.

Special Topics in Multi-component Decision Problems, by J. Van Ryzin. A series of eight lectures. Dept. of Statistics, Stanford University, Stanford, California, May 1967.

Spark Chamber Film Measuring Using the CHLOE System, by D. Hodges. University of Maryland, College Park, Maryland, June 1, 1967.

Mathematics Film Series

A number of films from the MATHEMATICS TODAY series were shown in the Applied Mathematics Division during the past year. Films in the series feature leading mathematicians discussing their specialties. The schedule was as follows:

November 8, 1966	Predicting at Random, a lecture by David Blackwell.
November 15, 1966	What is Mathematics and How Do We Teach It? A panel discussion with Lipman Bers, Samuel Eilenberg, Andrew Gleason, Henry Pollak, and Leo Zippin.
November 22, 1966	Challenging Conjectures, a lecture by R. H. Bing.
November 29, 1966	Gottingen and New York - Reflections on a Life in Mathematics, Richard Courant.
December 6, 1966	Challenge in the Classroom, the methods of R. L. Moore.
January 10, 1967	Pits, Peaks, and Passes, a lecture on critical point theory by Marston Morse. Parts I and II.
January 17, 1967	Can You Hear the Shape of a Drum? a lecture by Mark Kac.
January 24, 1967	The Classical Groups as a Source of Algebraic Problems, a lecture by Charles Curtis.
January 31, 1967	Applications of Group Theory in Particle Physics, a lecture by Freeman Dyson.
May 9, 1967	John von Neumann, a documentary on his life and work.